Analysis of gas dynamic waves in explosively actuated valves

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ANALYSIS OF GAS DYNAMIC WAVES IN EXPLOSIVELY ACTUATED VALVES

A Thesis

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
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in

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by

Blaise H. Paul
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Dedication

This work is dedicated to my wife Colleen, and to my parents Gary and Tammy. I thank my wife for her devotion and support throughout the completion of my academic endeavors, and I thank my parents for their constant encouragement and life lessons through example.
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I would like to thank the individuals who have contributed in various ways towards the completion of this work. First, I thank the Los Alamos National Laboratory (LANL), W-7 Division, Gas Transfer Systems (GTS) Group, and the W-6 Division, Detonator Design (DD) Group for financially supporting my work. There are numerous LANL employees who made this work possible, including Jay Carnes, W-7 GTS group leader; Derrick Montoya, W-6 DD group leader; Bob Nolen and Nathan Burnside, who were my LANL mentors; Manny Tafoya and Jose Tafoya, who generated experimental data; Michele Decroix, who truly made my stay at Los Alamos a smooth transition and an enjoyable experience; and Brett Okhuysen, who helped me gain an understanding in numerical methods, gas dynamics, and Linux operating systems.

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Abstract

A mathematical model is formulated for assessing quasi-one-dimensional gas dynamics occurring within axis-symmetric explosively actuated valves. The model describes complete valve operation and accounts for pressure-dependent explosive combustion within an actuator, compressible product gas flow within the actuator, through a small port, and into and within a gas expansion chamber. The gas dynamic waves induce piston motion at the terminal end of the expansion chamber which is needed for valve operation. The model is mathematically posed as an initial-boundary-value problem in terms of generalized coordinates to facilitate numerical computations on a domain that volumetrically expands due to combustion and piston motion. The model equations are numerically integrated using a total variation diminishing (TVD), high resolution shock capturing method.

Key objectives of this work are to characterize the influence of gas dynamic waves on device operation and performance, including the pyrotechnic shock transmitted to the valve’s supporting structure. For a baseline valve configuration, predictions give results that agree with experimental data for the expansion chamber pressurization rate, and both piston stroke time and velocity. The model is used to assess how variations in port cross-sectional area, explosive mass, geometric size, and other system parameters affect performance. This sensitivity analysis has shown, in all cases considered, that the pressurization rates of the actuator and the expansion chamber are the main factors that effect valve performance. High actuator pressurization rates are necessary for complete explosive combustion while high expansion chamber pressurization rates are necessary for rapid, monotonically increasing piston velocity that is desirable in practice.
Chapter 1
Introduction

Explosively and pyrotechnically actuated devices safely and reliably deliver high mecha-
nical power in remote locations. During combustion of the self-contained solid energetic, large
power output is achieved by the rapid production of gas which is used to perform work. These
devices are commonly applied in the aerospace industry due to their dependability, small size,
light weight, and long shelf life [41, 67]. Pin pullers, valves, thrusters, and cable cutters are
only a few examples of these devices that carry out critical functions such as chute deployment,
fluid flow control, jettison of components, and attitude control [12, 19, 41]. A summary and
background of these types of devices can be found in Refs. [10, 57, 65, 67].

During actuation, the combustion gas products generate large amplitude and high fre-
quency stress waves throughout the device’s mechanical components. These waves transmit
a pyrotechnic shock to the device’s surrounding support structure that must be considered in
device design and in selecting the appropriate device for a specific task [3]. An introduction
to pyrotechnic shock phenomena with an extensive bibliography can be found in Refs. [3, 77].

Historically, assessing device performance has been time consuming and expensive, and has
been heavily based on empiricism [11]. Although experiments are necessary to observe actual
device behavior, computational modeling can facilitate interpretation of experimental results
and can assist in the design of new and modified devices. In this study, a comprehensive, but
simple, mathematical model is formulated that can be used to examine the effects of geometric,
structural, and energetic material design modifications on both the performance of explosively
actuated devices and the pyrotechnic shock produced during actuation.

In the remainder of this chapter, a description of the model problem, the motivation for
this study, and a brief literature review are discussed. Lastly, the goals of this study are
specified and an outline of this thesis is given.

1.1 Problem Description and Research Motivation

The focus of this study is to mathematically and computationally examine the operation
and performance of a conventional nitrogen cartridge valve, but the model could be easily
adapted and applied to other devices such as pin pullers and cable cutters. Here, performance
collectively refers to quantities that are typically used to characterize valve operation such as its pressure history, piston velocity history, piston stroke time, and pyrotechnic shock. A schematic representing the nitrogen cartridge valve under consideration is shown in Fig. 1.1 in its prefired and postfired states. Also, an axial cross section of an actual nitrogen cartridge valve in its postfired state is shown in Fig. 1.2. The sole purpose of this valve is to quickly release stored nitrogen gas without contamination from the explosive combustion products. The valve is driven by the combustion of 150 mg of solid HMX (Her Majesty’s Explosive) explosive ($\ce{C4H8N8O8}$) which is contained within the actuator. The actuator threads into the expansion chamber which contains an initially tapered, 8.0 g piston. The piston is used to extract work from the system and complete the mechanical task. A port connects the actuator and expansion chamber, and initially supports a metal burst disc which hermetically seals the energetic from the surroundings and facilitates rapid combustion of the energetic material.

In order for the valve to properly function, a sequence of events must occur. First, the granular HMX explosive is remotely ignited by an embedded current carrying ignition wire. Rapid actuator pressurization occurs as the burst disc confines combustion within the actuator. The burst disc ruptures at approximately 50 MPa which allows combustion product gas
Figure 1.2: Actual cross-section of the explosively actuated nitrogen cartridge valve in its postfired state.

flow, and possibly burning solid explosive, through the port and into the expansion chamber. The pressure within the expansion chamber rises as combustion gas products are transported through the port. The high gas pressure pushes the piston down the expansion chamber performing work. As the piston is pushed down the bore, it deforms and creates a tight seal between the piston and bore thereby confining the gas within the actuator and expansion chamber. Additionally, the cutter located on the end of the piston punctures the diaphragm that contains the stored nitrogen gas. Once the diaphragm is punctured, the nitrogen gas is released and transferred through the conduit, as seen in Fig. 1.1(b). The piston reaches the stops, or completes its stroke, approximately 90 \( \mu s \) following ignition thus completing the function of the valve.

The possible need for a gas dynamic analysis is justified by comparing representative acoustic time scales with the device operational time. For instance, the nitrogen cartridge valve is characterized by the actuator and expansion chamber diameters, \( D_a \) and \( D_{ec} \), the actuator and expansion chamber lengths, \( L_a \) and \( L_{ec} \), and the port diameter, \( D_t \). These dimensions define longitudinal acoustic time scales for the actuator and expansion chamber, \( \tau_a = L_a/c_a \) and \( \tau_{ec} = L_{ec}/c_{ec} \), respectively, where \( c_a \) and \( c_{ec} \) are representative acoustic wave speeds. If
the valve actuation time is given by $\tau_v$, then spatial non-equilibrium effects associated with wave propagation are unimportant for $\tau/\tau_v \ll 1$, where $\tau$ are the acoustic time scales. For valves of interests to this study, $D_a \approx L_a \approx 5 \text{ mm}$, $D_{ec} \approx L_{ec} \approx 20 \text{ mm}$, $\tau_a \approx 3 \mu s$, $\tau_{ec} \approx 20 \mu s$, and $\tau_v \approx 90 \mu s$. Therefore, $\tau_a/\tau_v \approx 0.033$ and $\tau_{ec}/\tau_v \approx 0.222$. These estimates indicate that wave propagation may influence device performance.

Also indicated in Fig. 1.1(a) is the structural support that holds the valve in place and absorbs the pyrotechnic shock generated during actuation. Due to the combustion product gas waves, stress waves are generated within the valve’s mechanical components including the piston, actuator, and expansion chamber housing. Stress waves are also generated mechanically throughout the valve by piston-housing interference. The resulting stress waves from these interactions are transmitted to the structural support and collectively make up the pyrotechnic shock. The pyrotechnic shock is difficult to predict because of the complex wave interactions which are dependent on the explosive combustion process, valve geometry and material properties. It should be noted, however, most of the pyrotechnic shock is in the axial direction due to the axis-symmetric valve geometry.

In order to understand the complex nature of the pyrotechnic shock, its root cause must first be characterized. It is the gas dynamic pressure waves that induce deformations, and thus stress waves, within the valve’s solid components which are subsequently transmitted to the supporting structure. The gas dynamics not only drives, but is also largely independent of the solid mechanics because the solid deformations are small and only slightly modify the gas volume. Therefore, a gas dynamics analysis alone can give leading order information about pyrotechnic shock.

Additionally, there have been reported instances of explosively actuated device failures [5, 8]. Pyrotechnic shock induced failures of brittle components and electrical equipment, such as relays, switches, and glass diodes, have also been reported [50]. It is important to minimize failure rates because of the critical functions that these devices perform. Modeling, coupled with experiments, can lead to a better understanding of how these types of devices operate, and can reduce failures through improved designs and production decision making.

1.2 Literature Survey

In this section, experimental and modeling work relevant to this study are briefly discussed.
1.2.1 Experimental

As previously mentioned, experimental work has been the primary means of determining device performance in past years. The weight drop test is one of the earliest developed test that quantifies the energy input needed for device function [11]. For instance, consider the nitrogen cartridge valve as an example. The minimum energy required for valve actuation is determined by dropping a known mass from a measured height directly onto the piston. The minimum initial height of the falling mass, and thus the minimum gravitational potential energy, that results in complete piston stroke estimates the energy requirement for successful valve operation. Although the falling mass closely replicates the impulsive input of a solid energetic, the weight drop test is expensive since numerous single-use devices are consumed in obtaining the data.

Closed bomb tests are commonly conducted to determine the pressure rise and energy output that a given explosive or pyrotechnic actuator can produce. An actuator is fired into a constant volume chamber, usually 10 cc, and pressure-time data is measured using pressure transducers. Closed bomb test, while useful and easy to conduct, do not account for device volume changes associated with pin or piston motion. Other tests have been developed to account for such events including the Dynamic Test Device and the Variable Explosive Chamber (VEC) test [6, 55]. Velocity measurements of mechanical components, such as pins and pistons, have been obtained using Velocity Interferometer System for Any Reflector (VISAR) technology [2]. VISAR experiments utilize a laser beam, which must come in contact with the mechanical component, for data acquisition and are extremely accurate when correctly implemented.

The pyrotechnic shock generated during device operation is experimentally measured with accelerometers, strain gages, and laser Doppler vibrometers (LDV) [3]. LDV provides velocity measurements in isolated directions using a laser beam. Once pyrotechnic shock time-history data is obtained, a Shock Response Spectrum (SRS) can be generated to quantify the damage potential of a pyrotechnic shock [26]. The shock spectrum is a plot of the system’s maximum response as a function of its own natural frequency, and is commonly used in the design of structures that absorb pyrotechnic shock. Various tests have also been developed using shock spectrum to simulate pyrotechnic shock environments.
In recent years, a gas gun system has been developed and utilized at Los Alamos National Laboratory (LANL) that provides a relatively inexpensive and repeatable driving energy that better replicates actual loading conditions than the weight drop test [23, 69, 70]. The gas gun system has proved useful in determining work requirements for successful device operation and piston velocity measurements using VISAR. Also at LANL, non-intrusive diagnostic tests have been conducted with accelerometers and strain gages to assess device performance [51]. Unlike closed bomb and VISAR experiments, non-intrusive diagnostic tests enable evaluation of device performance without altering the device in any manner. Data is obtained by externally mounting accelerometers and strain gages to the device’s housing. While relatively easy to conduct, assessing device performance through these tests is challenging because of the complex acoustic wave interactions within the combustion gas products, and between the gas products and the device’s solid components.

1.2.2 Modeling

Ng developed one of the earliest models for explosively actuated devices called MAVIS [53]. The MAVIS model focuses on describing the piston dynamics for a valve that enables fluid flow by shearing tubes. Piston resistance is due piston-housing friction, tube cutting, and compressed gas pressure in front of the piston. Piston-housing deformations were assumed to be completely elastic until the emergence of the extended model MAVIS II, which accounts for plastic deformations as well [56]. In both MAVIS and MAVIS II, mass and energy release due to the combustion process are not explicitly modeled, but rather an empirically determined equation of state is used to describe the pressure that drives piston motion. Similarly, the work of Emery and Jones, et al [25, 35], describes the work required to move a piston within an explosively actuated valve. Their model accounts for piston resistance due to friction and geometrical interference, and elastic-plastic deformations with strain hardening effects. These models, while useful with respect to the piston and housing structural mechanics, do not consider the dynamic effects of mass and energy release and transport associated with the combustion process, or the effects of internal gas pressure on device deformation.

On the other hand, the work of Gonthier, et al [32], considered the thermochemistry of a pin puller. Their model includes the time-dependent mass and energy release of a pyrotechnic into gas and condensed phase products. This model accounts for volume changes due to pin motion,
and heat transfer between products and to the surroundings. Pin resistance during motion and device deformation are not, however, considered in the model. By incorporating coupled combustion and device deformation, Braud, et al [14, 15], have constructed a model that assesses the time-dependent, system-level response of explosively actuated valves. This model accounts for burning of a solid explosive to form product gas within an actuator, transport of product gas from the actuator to an expansion chamber, and insertion of an initially tapered piston into a constant diameter bore by gas pressure within the expansion chamber. Piston resistance is modeled similarly to the work of Ng [53, 56] and Emery, et al [25, 35], with the addition of resistance induced by internal gas pressure. Other noteworthy models include the work of Kuo, et al [38], for pin pullers, and the work of Butler, et al [17], and Vorozhtosov, et al [73], for airbag systems.

All of the models mentioned above that do incorporate combustion assume that acoustic time scales are much smaller than the devices operation time. This results in time-dependent, spatially homogeneous thermodynamic fields that can be described by a system of ordinary differential equations (ODEs). These models are incapable of predicting temporal fluctuations in pressure arising from acoustic wave interactions within the combustion product gases, and between these gases and the surrounding valve structure. The work of Lee [44], on the other hand, considers the unsteady effects of gas dynamic waves on device performance. This one-dimensional model includes momentum and energy interactions with the surroundings due to fluid-wall friction and heat transfer, and volume changes associated with piston motion. Lee demonstrated differences between an equilibrium and a gas dynamics model, and derived a nondimensional time parameter, similar to that presented earlier in Section 1.1, that can be used to determine if the unsteady gas dynamic effects are negligible. Lee’s model, however, does not include the mass and energy production from explosive combustion, but rather imposes a high pressure discontinuity as an initial condition to simulate combustion.

In recent years, miniaturization of explosively actuated devices has been explored to accommodate smaller systems which reduce payload and mission cost [60, 72]. The work of Rossi, et al [61, 62, 63], has been one of the forerunners in this research area with focus on microthrusters for satellite attitude control. Gonthier, et al [33], have explored performance variations for explosively actuated micro-valves using the previously mentioned model
of Braud, et al [14, 15]. In their work, a range of small scale valves with geometric similarity was considered, and three scale-dependent performance levels were identified. A similar study is presented in this work as discussed later in Section 4.3.

1.3 Objectives of This Study

The primary objective of this thesis is to formulate a comprehensive, but simple, mathematical model that can be used to examine the effect of design modifications on device performance and on the produced pyrotechnic shock. The model includes a gas dynamics analysis with features that have not been considered by others, including: 1) gas dynamic wave interactions with the combustion process and piston motion, 2) piston dynamics coupled with device elastic-plastic deformation, 3) device cross-sectional area variations, and 4) gas volume changes due to solid explosive combustion and piston motion. Specific objectives of this work are:

1. To predict the gas dynamic wave interactions within explosively actuated devices, and to identify their influence on both the explosive combustion process and piston motion.
2. To predict the leading order pyrotechnic shock produced during actuation of axis-symmetric explosively actuated devices.
3. To identify the influence of physical design parameters, such as geometry and explosive mass, on the operation and performance of explosively actuated devices.
4. To investigate the performance of geometrically similar, miniaturized explosively actuated devices.

Objective 1 is potentially important for the nitrogen cartridge valve since its performance may be governed by gas dynamic effects, as mentioned in Section 1.1. The gas pressure fields are of specific interest because the explosive combustion process is primarily pressure dependent, and the piston is driven by the high gas pressure that acts on its surface. Objective 2 is important because it gives insight as to what loading conditions the supporting structure will experience during device actuation. In addition, Objective 2 may also help in understanding the experimental results obtained from non-intrusive diagnostic tests conducted at LANL. From a design perspective, Objective 3 is important in obtaining devices with specific and optimal characteristics, and in determining the adverse effects of modifications on existing and well-established devices. Lastly, Objective 4 is important since smaller systems are
being considered that will likely include miniaturized explosively actuated devices. Although all proposed objectives could be accomplished through experiments, the developed model can produce results in a shorter time period with fewer financial costs. Furthermore, the model is another tool that can be utilized to investigate explosively actuated devices from a different perspective. The model is not, however, a substitute for experiments. A reduced set of experiments are still necessary to study and observe actual device performance, and validate the model’s predictions.

An outline of this paper is as follows. The time-dependent, quasi-one-dimensional model with assumptions, governing equations, initial conditions, and boundary conditions is first posed in Chapter 2. Next, in Chapter 3, the initial-boundary-value problem (IBVP) describing valve operation is transformed into generalized coordinates to facilitate its numerical integration. In addition, the numerical integration strategy is discussed, and simple problems with analytical solutions are simulated for model verification. In Chapter 4, baseline valve predictions are presented and comparisons are made with experimental data. A parametric analysis is conducted to investigate model sensitivity to parameters associated with the constitutive theory, and valve performance sensitivity to parameters of design importance. Miniaturized valve predictions are also presented and discussed in this chapter. Lastly, conclusions and recommendations for future work are summarized in Chapter 5.
Chapter 2
Mathematical Model

Accurately modeling the complete operation of the nitrogen cartridge valve is a difficult task because of the complex interplay between multi-phase combustion, product mass and acoustic energy transport, structural mechanics, and valve geometry. In this chapter, a simple model is formulated to account for the production and flow of an inert product gas that performs work in moving the piston. The model describes 1) pressure-dependent combustion of a granular solid explosive, 2) acoustic mass and energy transport within and between the actuator and expansion chamber, and 3) piston motion within the expansion chamber bore. Piston motion is driven by high pressure gas acting on its surface, and is opposed by resistance induced by piston-housing friction and geometrical interference. Importantly, key geometrical features of the valve are retained, including: 1) cross-sectional area variations with axial position, 2) volume changes within the actuator due to solid combustion, and 3) volume changes within the expansion chamber due to piston motion. Figure 2.1 illustrates the simplified nitrogen cartridge valve with these key model features.

The nitrogen cartridge valve is modeled as quasi-one-dimensional since it exhibits axis-symmetrical geometry. By approximating the valve as quasi-one-dimensional, the model re-
tains the simplicity of a one-dimensional model while still capturing important features of the valve such as mass choking through the port. The quasi-one-dimensional assumption is valid for small, continuous changes in cross-sectional area; as such, the abrupt area changes near the port are smoothed out for the analysis. Also, the cross-sectional area variations corresponding to the tapered region of the expansion chamber, which is used to initially support the piston (see Fig. 1.1(a)), are ignored in the analysis. The area variations are small in this region and are assumed to have a negligible effect on the gas dynamics. Therefore, the expansion chamber is modeled as having a constant cross-sectional area beyond the port region. The tapered region of the expansion chamber does, however, play an important role in piston resistance due to geometrical interference. This interference between the piston and expansion chamber bore is accounted for in the model, and has a large effect on valve performance, as demonstrated in Section 4.1.1.

The combustion of solid HMX forms multiple gas phase product species [71]. Here, details of the chemical kinetics are ignored and the gas is modeled as ideal with properties that are representative of HMX combustion products. Furthermore, the burst disc is neglected in the analysis although it may have an effect on valve performance as discussed later in Chapter 5. Additional simplifications and assumptions are explained as each model feature is discussed in more detail.

A convenient system decomposition for describing the model is shown in Fig. 2.2. The combustion product gas is confined to the domain \(-L_e(t) \leq x \leq L_p(t)\), respectively, where \(L_e(t)\) and \(L_p(t)\) are the instantaneous locations of the explosive and piston boundaries. The explosive combustion process and piston dynamics are imposed at these boundaries. Volume changes within the valve are accounted for as these boundaries move axially with time. The explosive boundary advances within the actuator as solid explosive is consumed by combustion, and the piston boundary advances as the piston moves within the expansion chamber bore.

The remainder of this chapter is as follows. In Section 2.1, the theoretical formulation and model equations are given. The explosive and piston boundary conditions are then formulated in Section 2.2. Lastly, in Section 2.3, a mathematical expression for the pyrotechnic shock is formulated.
2.1 Model Equations

Equations governing the evolution of combustion product gas mass, momentum, and energy within the domain $-L_e(t) < x < L_p(t)$ are classical, and are respectively given by the Euler equations of gas dynamics with cross-sectional area variations [68]:

\[
\frac{\partial}{\partial t} (A\rho) + \frac{\partial}{\partial x} (A\rho u) = 0, \tag{2.1}
\]

\[
\frac{\partial}{\partial t} (A\rho u) + \frac{\partial}{\partial x} [A (\rho u^2 + p)] = p \frac{dA}{dx}, \tag{2.2}
\]

\[
\frac{\partial}{\partial t} (A\rho E) + \frac{\partial}{\partial x} \left[ A\rho u \left( E + \frac{p}{\rho} \right) \right] = 0. \tag{2.3}
\]

Independent variables appearing in these equations include time $t$ and axial position $x$. Dependent variables include gas density $\rho$, velocity $u$, pressure $p$, and total specific energy $E = e + u^2/2$, where $e$ is mass specific internal energy. The term on the right hand side of Eq. (2.2) represents an axial momentum exchange with the surroundings induced by pressure interactions along the curved surface of the device wall. Due to the valve’s fast operation time, heat transfer effects to the surroundings are small and are ignored in the analysis. The axial variation in device cross-sectional area $A(x)$ is a prescribed function of position and is loosely representative of the actual nitrogen cartridge valve. Moving the area terms to the right hand side of the equality in Eqs. (2.1)-(2.3), and rearranging terms, results in
\[ \frac{\partial}{\partial t} (\rho) + \frac{\partial}{\partial x} (\rho u) = -\rho \frac{1}{A} \frac{dA}{dx}, \]  \hspace{1cm} (2.4) \\
\[ \frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2 + p) = -\rho u \frac{1}{A} \frac{dA}{dx}. \]  \hspace{1cm} (2.5) \\
\[ \frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x} [\rho u (E + \frac{p}{\rho})] = -\rho u \left( E + \frac{p}{\rho} \right) \frac{1}{A} \frac{dA}{dx}. \]  \hspace{1cm} (2.6)

The above form of the governing equations is preferred in this work since the valve’s cross-sectional area is a prescribed function of position. The spatial derivative of \( A \) can be directly evaluated rather than numerically approximated thus making the model’s predictions more accurate. The thermal and caloric equations of state for the gas are ideal, and are given by

\[ p = p(\rho, T) = \rho RT, \]  \hspace{1cm} (2.7) \\
\[ e = e(T) = c_v T, \]  \hspace{1cm} (2.8)

respectively, where \( R \) is the gas constant and \( c_v \) is the constant volume specific heat; the values for \( R \) and \( c_v \) were chosen to match values for HMX product compositions predicted by the CHEMKIN thermochemistry package. A brief summary of the CHEMKIN analysis and results are presented in Appendix A.

Equations (2.4)-(2.8) constitute a system of five equations with five unknowns (i.e., \( \rho, u, e, p \), and \( T \)); thus the system is mathematically closed. Initial conditions prescribed over the domain \( L_e^0 \leq x \leq L_p^0 \), where \( L_e^0 \) and \( L_p^0 \) are the initial boundary locations, are given by

\[ p(x, 0) = p^0, \quad T(x, 0) = T^0, \quad u(x, 0) = 0, \]  \hspace{1cm} (2.9)

and the gas equations of state are used to evaluate \( \rho^0 = \rho(p^0, T^0) \) and \( e^0 = e(T^0) \). The solution to the system of equations with the above initial conditions can be determined once the boundary conditions are supplied.

### 2.2 Boundary Conditions

The explosive and piston boundary conditions are imposed at \( x = -L_e(t) \) and \( x = L_p(t) \), respectively, as illustrated in Fig. 2.2. In this section, a simple combustion model for the explosive boundary, and the dynamics for the piston boundary, are described and formulated.
2.2.1 Explosive Combustion

Product gas mass, momentum, and energy fluxes imposed at the explosive boundary are determined based on a simple combustion model. To this end, it is assumed that the ignition process, triggered by an embedded hot wire in practice, occurs quickly and uniformly throughout the explosive producing $N_e$ simultaneously burning spherical grains within the combustion zone, as depicted in Fig. 2.3(a). It is further assumed that the combustion zone is well-stirred so that no spatial variations exist in explosive and gas properties. Thus, ignoring kinetic energy changes, the evolution of mass and energy for the solid explosive and product gas contained within the combustion zone can be described by

\begin{align}
\frac{d}{dt}(\rho_e \phi_e V_c) &= -\rho_e A_e r_e, \quad (2.10) \\
\frac{d}{dt}(\rho_g \phi_g V_c) &= \rho_e A_e r_e - \dot{m}_g, \quad (2.11) \\
\frac{d}{dt}(\rho_e \phi_e V_e e_e) &= -\rho_e A_e r_e e_e, \quad (2.12) \\
\frac{d}{dt}(\rho_g \phi_g V_e e_g) &= \rho_e A_e r_e e_e - \dot{m}_g \left( e + \frac{p}{\rho} + \frac{u^2}{2} \right). \quad (2.13)
\end{align}

Here, explosive properties are denoted by subscript “e” and gas properties contained within the combustion zone are denoted by subscript “g”. Forcing terms in Eqs. (2.10)-(2.13) account for mass and energy exchange between the explosive and gas due to combustion, and flow of gas mass and energy through the explosive boundary into the actuator volume as shown in Fig. 2.3(b). It is noted that all explosive mass is confined to the combustion zone within the context of this model. New variables introduced in these equations include the explosive and gas volume fractions $\phi_e = V_e/V_c$ and $\phi_g = V_g/V_c$, the combustion zone volume $V_c$, the explosive burn rate $r_e$, the explosive burn surface area $A_e$, and the product gas mass flow rate through the explosive boundary $\dot{m}_g$, where $\dot{m}_g = \rho u A_a$, and $A_a$ is the cross-sectional area of the actuator chamber. From mixture theory, the explosive and gas products within the combustion zone are constrained by the saturation condition:

$$\phi_e + \phi_g = 1, \quad (2.14)$$
which states that the combustion zone volume is completely occupied by the explosive-gas mixture. The combustion zone volume decreases with time as the solid energetic burns with gas products transported across the explosive boundary. Using simple geometric relations, the time-dependent combustion zone volume can be described by

\[ V_c(t) = A_a(L_a - L_e(t)), \] (2.15)

where \( L_a \) is the constant axial length of the actuator chamber. As commonly done, the explosive burn rate is taken to be pressure dependent. Expressions for the explosive burn rate, radius of a single burning grain, and the total explosive burn surface area are given by

\[ r_e \equiv \frac{dR_e}{dt} = a p^n, \quad R_e = \left( \frac{3\phi_e V_c}{4\pi N_e} \right)^{1/3}, \quad A_e = 4\pi R_e^2 N_e, \] (2.16)

where \( a \) and \( n \) are material dependent and empirically determined combustion constants. The explosive is assumed incompressible (i.e., \( \rho_e = \rho_e^0 \)) and heat interactions between the explosive and product gas are ignored. As such, it can be shown by multiplying Eq. (2.10) by \( e_e \), and subtracting the resulting expression from Eq. (2.12), that the specific internal energy of the explosive is constant during combustion (i.e., \( e_e = e_e^0 \)).

For simplicity, it is further assumed that \( \phi_g \ll 1 \) for all time within the combustion zone. Therefore, to leading order, \( \phi_g \approx 0 \) and \( \phi_e = 1 - \phi_g \approx 1 \) from the saturation condition given by Eq. (2.14). Substituting \( \phi_e \approx 1 \) and the geometrical relation for \( V_c \) into Eq. (2.10), and rearranging the resulting expression gives

\[ \frac{dL_e}{dt} = \frac{A_e}{A_a} r_e, \] (2.17)

which describes the time-dependent location of the explosive boundary. The initial condition to Eq. (2.17) is \( L_e(0) = L_e^0 \). In this limit (\( \phi_e \approx 1 \)), the radius of an explosive grain and the total burn surface area reduce to

\[ R_e(t) = \left[ \frac{3A_a(L_a - L_e(t))}{4\pi N_e} \right]^{1/3}, \quad A_e(t) = 4\pi R_e(t)^2 N_e. \] (2.18)
It is noted that Eq. (2.17) depends on the product gas pressure at the explosive boundary through the burn rate $r_e(p)$; this pressure is numerically estimated based on linear extrapolation of pressure from within the product gas computational domain, as explained in the following chapter. Consequently, product gas pressure waves occurring within the actuator chamber can influence explosive combustion.

Likewise, substituting $\phi_g \approx 0$ in both Eqs. (2.11) and (2.13), and rearranging the resulting algebraic constraints gives the gas mass and energy fluxes at the explosive boundary

\[
\rho u = \frac{\dot{m}_g}{A_a} = \frac{\rho_e^0 A_e r_e}{A_a},
\]

\[
\rho u (e + \frac{p}{\rho} + \frac{u^2}{2}) = \frac{\rho_e^0 A_e r_e q}{A_a},
\]

where $q \equiv \epsilon_e^0$ is the specific combustion energy of the explosive. Equations (2.19) and (2.20) contain the four unknowns $\rho$, $u$, $e$, and $p$. Given the product gas pressure at the explosive boundary $p$, and using the gas equations of state given by Eqs. (2.7) and (2.8), then Eqs. (2.19) and (2.20), can be combined to obtain a quadratic expression for $\rho$:

\[
\rho^2 - \frac{p}{q} \left( \frac{\gamma}{\gamma - 1} \right) \rho - \frac{1}{2q} \left( \frac{\rho_e^0 A_e r_e}{A_a} \right)^2 = 0.
\]
Numerical simulations indicate that only one root of this expression is non-negative and, thus, physically meaningful. Corresponding values for \(u(\rho, p)\) and \(e(\rho, p)\) can then be evaluated from Eqs. (2.19) and (2.20). The product gas momentum flux at the explosive boundary is then specified by \(\rho u(\rho, p)^2 + p\). Once combustion is complete at time \(t_{\text{burn}}\), \(L_a(t) = L_a\) and the boundary is switched to a zero mass flux condition which requires \(u(L_a, t) = 0\) for \(t \geq t_{\text{burn}}\) corresponding to a reflective wall.

### 2.2.2 Piston Dynamics

The piston moves in response to the gas dynamic pressure force that drives motion and the resistive force which opposes motion. Newton’s law of motion for the piston is given by

\[ m_p \frac{d^2}{dt^2} (L_p) = F_p - F_R, \]  

(2.21)

where \(L_p(t)\) is the axial location of the piston, \(m_p\) is the piston mass, \(F_p\) is the gas dynamic pressure force, and \(F_R\) is the piston resistance force. The actual piston has a complex geometry within its hollow region, as illustrated by Fig. 1.2. For simplicity, the complex cross-sectional area variations associated with the hollow piston geometry are ignored, and the piston is modeled as a flat disc. Therefore, the pressure force that acts on the piston surface is evaluated by

\[ F_p(t) = p(L_p(t), t)A_p, \]  

(2.22)

where \(A_p = \pi D_{cc}^2/4\) is the constant piston cross-sectional area. The tapered region and piston thickness are, however, important in determining the resistive force, and are accounted for by the piston-housing deformation model developed by Braud, et al [14, 15]. In this thesis, the piston-housing deformation model is referred to as the piston resistance model since it is utilized for evaluating the resistive force only. Here, only the key features of the piston resistance model that are relevant to this work are briefly discussed; the cited references should be consulted for a complete derivation and discussion.

The piston resistance model is largely based on cylindrical pressure vessel theory. The resistive force is determined from the interface stress between the piston and housing, and is dependent on both the piston and housing material properties. The interface stress is induced
by geometrical interference and internal gas pressure that acts throughout the hollow piston. Within the context of this study, the pressure that acts throughout the hollow piston is taken as the pressure at the piston boundary \( p(L_p(t), t) \). This is a reasonable approximation since the axial depth of the piston’s tapered region is relatively shallow. Figure 2.4 is a drawn to scale illustration of the hypothetical piston used in the gas dynamics and piston resistance model formulation at its initial position.

![GAS DYNAMICS MODEL](image1)

![PISTON RESISTANCE MODEL](image2)

Figure 2.4: Illustration of the hypothetical piston used in the gas dynamics and piston resistance model formulations; each piston is drawn to scale.

In the piston resistance model, the hollow portion of the piston is assumed to initially lie completely in the tapered region of the expansion chamber. Only the hollow section of the piston is assumed to contribute to piston resistance; the remaining solid portion is frictionless and contains the remaining mass. As gas pressure begins to act on the piston, part of the hollow region will be pushed into the bore while the rest will remain in the tapered region. For this reason, the resistive force is broken into two components. The hollow portion of the piston in the tapered section of the expansion chamber is referred to as the skirt region, while the remaining hollow portion of the piston is referred to as the bore region. Therefore, the resistive force is evaluated by

\[
F_R(t) = F_{skirt}(t) + F_{bore}(t).
\]  

(2.23)

Figure 2.5 indicates these different piston sections used in the piston resistance model formulation. Initially, \( F_{skirt} = F_{bore} = 0 \), and \( F_{skirt} \to 0 \) as the entire piston is pushed into
the bore. As the piston is acted upon by the gas, geometrical interference and internal gas pressure causes a compressive radial stress at the piston-housing interface (i.e., $\sigma_r = -\bar{P}$). It is assumed that this interface stress locally induces a tangential frictional stress, $\bar{\tau} = -\mu \bar{P}$, where $\mu$ is a constant coefficient of friction. Since interference varies with both axial position and time, $\bar{P} = \bar{P}(\lambda, t)$ and $\bar{\tau} = \bar{\tau}(\lambda, t)$, where $\lambda$ is an axial coordinate measured relative to the top of the piston, as illustrated in Fig. 2.6. The inner, interface, and outer radii at a given cross-section are given by $a(\lambda, t)$, $b(\lambda, t)$, and $c(\lambda, t)$, respectively. The resistive force components are therefore given by

$$F_{\text{skirt}}(t) = (\mu_s \cos \theta + \sin \theta) \int_{A_{\text{skirt}}} \bar{P}(\lambda, t) \, dA, \quad F_{\text{bore}}(t) = \mu_b \int_{A_{\text{bore}}} \bar{P}(\lambda, t) \, dA,$$  

(2.24)

where $\mu_s$ and $\mu_b$ are the coefficients of friction in the skirt and bore regions, and $\theta$ is the angle of piston taper measured relative to the axis of symmetry. The values of the coefficients of friction were determined through quasi-static compression test performed on actual nitrogen cartridge valves.

![Figure 2.5: Schematic of the piston regions used for establishing the piston resistance force.](image)

Each component is integrated over their interfacial surface area. Here, the piston skirt and bore region have the shape of a conical frustum and cylinder. Therefore, the integrals can be reduced to one-dimensional integrals in terms of $\lambda$:

$$F_{\text{skirt}}(t) = (\mu_s \cos \theta + \sin \theta) \int_0^{L-L_p(t)} \bar{P}(\lambda, t) \, g(\lambda, t) \, d\lambda,$$
Figure 2.6: Schematic of the coordinate system used for establishing the piston resistance force.

\[ F_{\text{bore}}(t) = 2\pi \mu_b R_b \int_{L-L_p(t)}^{L_p} \tilde{P}(\lambda, t) \, d\lambda, \tag{2.25} \]

where

\[
g(\lambda, t) = \pi \sqrt{[b(0, t) - b(\lambda, t)]^2 + \lambda^2} \left[ \frac{\partial b}{\partial \lambda} + \frac{[b(0, t) + b(\lambda, t)] \left( \lambda - [b(0, t) - b(\lambda, t)] \frac{\partial b}{\partial \lambda} \right)}{[b(0, t) - b(\lambda, t)]^2 + \lambda^2} \right],
\]

and

\[
b(\lambda, t) = \left[ \frac{R_b - b(0, t)}{L - L_p(t)} \right] \lambda + b(0, t).
\]

The constant radius bore region is given by \( R_b \). It is further assumed that the piston and housing only experience small deformations. Thus, the piston length \( \hat{L}_p \) remains constant since \( \theta \ll 1 \). To complete evaluating the resistive force components given by Eq. (2.25), the interface stress \( \tilde{P}(\lambda, t) \) must be calculated. The local interface stress is evaluated based on a steady, two-dimensional, elastic-plastic plane strain theory which assumes that the stress state rapidly equilibrates during piston motion. Details of the derivation and solution behavior are lengthy, and can be found in Refs. [14, 15].

Once the resistive and pressure forces are known, Eq. (2.21) can be solved to determine the piston’s position and velocity. The second-order ordinary differential equation (ODE) is first split into two first-order ODEs:
\[ m_p \frac{dv_p}{dt} = F_p - F_R, \quad (2.26) \]
\[ \frac{dL_p}{dt} = v_p, \quad (2.27) \]

where \( v_p(t) \) is the piston velocity. The initial conditions for these equations are \( v_p(0) = 0 \), and \( L_p(0) = L^0_p \). A zero mass flux condition is imposed on the product gas at the piston boundary which requires \( u(L_p(t), t) = v_p(t) \) until the piston reaches the stops. Once the piston completes its stroke at \( t = t_{stk} \), \( L_p(t) = L_{ec} \) and the zero mass flux condition is altered to \( u(L_{ec}, t) = 0 \) for \( t \geq t_{stk} \).

A completely defined IBVP is given by the governing PDEs, Eqs. (2.4)-(2.6), the equations of state, Eqs. (2.7)-(2.8), with initial conditions Eq. (2.9), and the previously described boundary conditions.

### 2.3 Pyrotechnic Shock

Peak forces transmitted to the supporting structure are expected to be in the axial direction due to the valve’s axis-symmetric geometry. Here, the dynamic stress waves within both the valve’s solid components and structural members are ignored, and the pyrotechnic shock is taken as the net axial force that acts on the valve’s housing. This time-dependent force is induced by the gas dynamics, and is evaluated by

\[ F_{pyro}(t) = F_a(t) + F_{p,a}(t) + F_{ec}(t), \quad (2.28) \]

where \( F_a(t) \) is the pressure force that acts on the actuator surface, \( F_{p,a}(t) \) is the net axial pressure force that acts on the curved surfaces of the valve, and \( F_{ec}(t) \) is the transmitted force that acts on the housing through piston contact. These forces are indicated in Fig. 2.7.

During the combustion process, the pressure force that acts on the actuator surface at \( x = -L_a \) is taken as the stagnation pressure since the velocity at this boundary is always zero. Therefore, the pressure force that acts on the actuator surface is given by

\[ F_a(t) = -p_0(t)A_a, \quad (2.29) \]
where the stagnation pressure $p_0$ within the combustion zone is given by

$$p_0(t) = p(-L_e(t), t) \left[ 1 + \frac{\gamma - 1}{2} Ma(-L_e(t), t)^2 \right]^\frac{\gamma}{\gamma - 1}, \quad (2.30)$$

and $Ma(-L_e(t), t)$ is the Mach number at the explosive boundary. Notice, once complete combustion occurs $Ma(-L_a, t) = 0$ such that $p_0(t) = p(-L_a, t)$.

The net axial pressure force that acts on the curved surface is obtained by integration. Using geometry and the spatial derivative of the valve diameter $D(x)$, the following expression is formulated:

$$F_{p,a}(t) = -\frac{\pi}{2} \int_{L_a(t)}^{L_p(t)} p(x, t) D(x) \frac{dD}{dx} dx. \quad (2.31)$$

Depending on the pressure field within the actuator and expansion chamber, this force will act in either the positive or negative direction. A complete derivation of Eq. (2.31) is given in Appendix B.

As the piston is pushed down the bore by gas pressure, both the piston and expansion chamber housing are subjected to the resistive force. With respect to the valve’s housing, the resistive force acts in the positive $x$-direction during piston motion. Once the piston reaches the stops, it comes to rest and a pressure force is transmitted through the stationary piston to the housing. Therefore, the force that acts on the housing from interactions with the piston is given by
\[
F_{ec}(t) = \begin{cases} 
F_R(t) & \text{for } t < t_{stk}, \\
p(L_{ec}, t)A_p & \text{for } t \geq t_{stk}.
\end{cases}
\] (2.32)

The instantaneous pyrotechnic shock, induced by the gas dynamics, is evaluated by Eq. (2.28) once the three force components are known.
Chapter 3
Numerical Method

In this chapter, the numerical method used to integrate the IBVP posed in the previous
chapter is described. First, in Section 3.1, the governing equations are transformed to a
generalized coordinate system to facilitate their numerical integration. Then, the technique for
numerically solving the transformed governing equations is described in Section 3.2. Lastly,
three problems with known analytical solutions are simulated for numerical verification in
Section 3.3.

3.1 Generalized Coordinate Transformation

To facilitate numerical integration of Eqs. (2.4)-(2.6) on the expanding domain \( L_e(t) \leq x \leq L_p(t) \), subject to flux conditions at the explosive and piston boundaries, these equations
are expressed in terms of generalized coordinates on a fixed computational domain. Figure
3.1 illustrates the computational grid for both the distorting time-dependent physical domain
\((x, t)\) and the fixed computational domain \((\xi, \tau)\).

A general coordinate transformation of the independent variables \((x, t) \rightarrow (\xi, \tau)\) requires

\[\xi = \xi(x, t), \quad \tau = \tau(x, t).\] (3.1)

The differential operators are determined by direct application of the chain rule:

\[\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial \tau}{\partial \xi} \frac{\partial \xi}{\partial \tau},\] (3.2)

\[\frac{\partial}{\partial t} = \frac{\partial \xi}{\partial \xi} \frac{\partial \xi}{\partial t} + \frac{\partial \tau}{\partial \xi} \frac{\partial \xi}{\partial \tau}.\] (3.3)

The terms \(\xi_x, \xi_t, \tau_x,\) and \(\tau_t\) denote partial derivatives with respect to the subscript variables,
and are referred to as the grid metrics. The coordinate transformation of Eq. (3.1) is given by
the algebraic expressions:

\[\xi = \xi(x, t) = \frac{x - L_e(t)}{L_p(t) - L_e(t)}, \quad \tau = \tau(x, t) = t,\] (3.4)
where $\xi \in [0, 1]$ and $\tau \in [0, \infty)$, respectively. The differential operators reduce to

\begin{align}
\frac{\partial}{\partial x} &= \xi_x |_t \frac{\partial}{\partial \xi}, \\
\frac{\partial}{\partial t} &= \xi_t |_x \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \tau} |_\xi,
\end{align}

where the grid metrics are given by

$$
\xi_x = \frac{1}{x_\xi}, \quad \xi_t = -\frac{x_\tau}{x_\xi}.
$$

The metric $\xi_x$ is the Jacobian which accounts for grid stretching. Both grid metrics can be evaluated either by direct differentiation of Eq. (3.4), or through finite differencing of Eq. (3.7) using the grid point locations in both coordinate systems. In this work, the grid metrics are evaluated by finite differencing in order to both generalize and modularize the computer algorithm for more complex transformations. Numerical simulations were conducted with the grid metrics evaluated by each of the two methods, and the results were indifferent.

Applying the differential operators given by Eqs. (3.5)-(3.6) to Eqs. (2.4)-(2.6), and rearranging the result, gives the governing equations in terms of the generalized coordinates:

\begin{align}
\frac{\partial}{\partial \tau} \left( \frac{\rho}{\xi_x} \right) + \frac{\partial}{\partial \xi} \left( \frac{\rho U_c}{\xi_x} \xi_x \right) &= -\rho u \frac{1}{A} \frac{\partial A}{\partial \xi}, \\
\frac{\partial}{\partial \tau} \left( \frac{\rho u}{\xi_x} \right) + \frac{\partial}{\partial \xi} \left[ \frac{1}{\xi_x} (\rho u U_c + \xi_x p) \right] &= -\rho u^2 \frac{1}{A} \frac{\partial A}{\partial \xi}, \\
\frac{\partial}{\partial \tau} \left( \frac{\rho E}{\xi_x} \right) + \frac{\partial}{\partial \xi} \left[ \frac{\rho}{\xi_x} \left( EU_c + \frac{\xi_x p}{\rho} \right) \right] &= -\rho u \left( E + \frac{p}{\rho} \right) \frac{1}{A} \frac{\partial A}{\partial \xi}.
\end{align}
The variable $U^c$ appearing in these equations is the contravariant velocity defined by

$$U^c = \xi_t + \xi_x u,$$  \hspace{1cm} (3.11)

which is the velocity of the gas in the $\xi$-direction. Eqs. (3.8)-(3.10) constitute a strictly hyperbolic system of partial differential equations; the eigenvalues of the generalized flux Jacobian matrix are both real and distinct, and are given by $U^c$, $U^c + \xi_x c$, and $U^c - \xi_x c$, where $c = \sqrt{\gamma RT}$ is the sound speed and $\gamma$ is the specific heat ratio. The generalized flux Jacobian is defined mathematically as $\frac{\partial f}{\partial q}$, and its corresponding eigenvalues are needed for the numerical technique as described in the following section. A complete derivation of the grid metrics, Eqs. (3.7), transformed governing equations, Eqs. (3.8)-(3.10), and the eigenvalues of the generalized flux Jacobian can be found in Appendix C.

The boundary conditions, established in the preceding chapter, are expressed in terms of the generalized coordinates by applying Eq. (3.6) to Eq. (2.17) for the explosive boundary, and to Eqs. (2.26)-(2.27) for the piston boundary. The resulting expressions are given by

$$\frac{dL_e}{d\tau} = \frac{A_e}{A_a} v_e,$$  \hspace{1cm} (3.12)

$$m_p \frac{dv_p}{d\tau} = F_p - F_R,$$  \hspace{1cm} (3.13)

$$\frac{dL_p}{d\tau} = v_p.$$  \hspace{1cm} (3.14)

Eq. (3.12) is imposed at $\xi = 0$, while Eqs. (3.13)-(3.14) are imposed at $\xi = 1$. Since $L_e(t)$, $v_p(t)$, and $L_p(t)$ are functions of time only, Eqs. (3.12)-(3.14) are identical to those expressed in the physical coordinate system.

### 3.2 Kurganov-Tadmor Technique

The fundamental conservation laws, given by Eqs. (3.8)-(3.10), are expressed as a system of partial differential equations in vector conservative form:

$$\frac{\partial}{\partial \tau} q(\xi, \tau) + \frac{\partial}{\partial \xi} f(q(\xi, \tau)) = w(q(\xi, \tau)),$$  \hspace{1cm} (3.15)

where $q \in \mathbb{R}^3$ is the conserved vector, $f(q) \in \mathbb{R}^3$ is the nonlinear convection flux vector, and
$w(q) \in \mathbb{R}^3$ is the source vector ($\mathbb{R}^3$ is a set of 3 real numbers). These vectors are given by

$$q = \begin{bmatrix} \rho, \rho u, \rho E \end{bmatrix}^T,$$

$$f(q) = \begin{bmatrix} \frac{\rho U^c}{\xi_x}, \frac{1}{\xi_x} (\rho u U^c + \xi_x p), \frac{\rho}{\xi_x} \left( E U^c + \frac{\xi_x p}{\rho} \right) \end{bmatrix}^T,$$

$$w(q) = \begin{bmatrix} -\rho u \frac{1}{A} \frac{\partial A}{\partial \xi}, -\rho u^2 \frac{1}{A} \frac{\partial A}{\partial \xi}, -\rho u \left( E + \frac{p}{\rho} \right) \frac{1}{A} \frac{\partial A}{\partial \xi} \end{bmatrix}^T.$$

In general, central-difference techniques can be implemented to numerically solve these types of problems in a fairly straightforward manner provided that appropriate attention is placed on numerical stability. In this work, a high resolution, total variation diminishing (TVD) numerical method is utilized which accurately captures shocks with minimal diffusion and dispersion.

The employed numerical method is an extension of the Lax-Friedrichs (LxF) technique, which is the forerunner and foundation of today’s advanced central-difference techniques [27, 42]. LxF is nominally first-order accurate in both time and space, and is relatively simple as compared to Godunov type techniques which require a characteristic based approach [30]. However, since LxF is only first-order accurate, large numerical viscosity occurs which prevents sharp resolution of large gradient phenomena such as shocks and contact waves. Later, the Nessyahu-Tadmor (NT) technique was developed from LxF where the order of accuracy in space is increased to second-order [52]. This method retains the simplicity of LxF while gaining resolution and reducing numerical viscosity. The resolution of NT was further enhanced by the extended Kurganov-Tadmor (KT) technique despite having the same nominal order of accuracy [39]. Sharper resolution is achieved by analyzing the smooth (continuous) and the non-smooth (discontinuous) portions of the solution separately. The smooth and nonsmooth solution regions are detected from the eigenvalues of the flux Jacobian. No other knowledge of the underlying eigenstructure is required making the method relatively simple to implement.

Furthermore, unlike LxF and NT, the KT fully-discrete technique admits a semi-discrete formulation where higher accuracy in time can be obtained.

In this work, the governing conservation equations given in vector conservative form by Eq. (3.15) are numerically solved using the KT semi-discrete technique with fourth-order Runge-
Kutta (4RK) for time integration. Thus, the gas dynamics model is nominally second-order accurate in space and fourth-order accurate in time. The semi-discrete, finite volume form of the conservation equations is given by

$$\frac{d}{d\tau} Q_j(\tau) = - \frac{F_{j+1/2}(\tau) - F_{j-1/2}(\tau)}{\Delta\xi} + W_j(\tau),$$  \hspace{1cm} (3.16)

where $Q_j(\tau)$ is a discretized vector approximation of the conserved vector $q(\xi = \xi_j, \tau)$, $F_{j+1/2}(\tau)$ and $F_{j-1/2}(\tau)$ are numerical flux vectors, and $W_j(\tau)$ is the discretized source vector corresponding to $w(\xi = \xi_j, \tau)$. An illustration of the finite volume at $(\xi = \xi_j, \tau)$ with these vectors are given by Fig. 3.2. The model equations are numerically solved on the fixed computational domain, which is discretized into $N_\xi$ evenly spaced cells of width $\Delta\xi = 1/N_\xi$, and the integration time increment $\Delta\tau$ is chosen based on a CFL (Courant Friedrichs Lewy) number of 0.40 for numerical stability. The boundary conditions given by Eqs. (3.12)-(3.14) are also numerically integrated in time using 4RK, and are updated in the gas dynamics algorithm in each of the four intermediate steps required to advance the solution over a time increment $\Delta\tau$.

The numerical technique requires spatial derivatives of the conserved vector $q(\xi, \tau)$. These derivatives are reconstructed from the computational cell averages using a $\theta$-dependent min-mod limiter. The employed limiter is generally less dissipative than the original minmod while retaining the TVD property. Spurious oscillations are minimized by investigating the smoothness of the solution through backward, central, and forward difference approximations. Spatial derivatives of $q(\xi, \tau)$ are evaluated by

$$\frac{\partial}{\partial\xi} q(\xi, \tau) \approx \text{minmod} \left( \theta \frac{Q_j(\tau) - Q_{j-1}(\tau)}{\Delta\xi}, \frac{Q_{j+1}(\tau) - Q_{j-1}(\tau)}{2\Delta\xi}, \theta \frac{Q_{j+1}(\tau) - Q_j(\tau)}{\Delta\xi} \right),$$  \hspace{1cm} (3.17)
where the minmod function is defined by

\[
\text{minmod} (d_1, d_2, d_3) = \begin{cases} 
\min (d_i), & \text{if } d_i > 0 \ \forall \ i \\
\max (d_i), & \text{if } d_i < 0 \ \forall \ i \\
0, & \text{otherwise.}
\end{cases}
\]

(3.18)

The parameter \( \theta \in [1, 2] \) is selected in an optimal manner such that sharp resolution without oscillations are obtained.

### 3.3 Verification Studies

Three example problems having analytical solutions were simulated to verify the numerical algorithm: 1) the classical shock tube problem, 2) steady flow through a Laval nozzle, and 3) unsteady expansion induced by two impulsively retracted pistons. Each problem is a special limiting form of the governing model equations and boundary conditions already given. The first two problems were chosen to separately verify the coupled space and time accuracy of the method and the effect of area variation on the solution for time-independent computational grids. For the third problem, the grid expands in time due to the retracting pistons; this problem was intended to verify the grid metrics implementation.

#### 3.3.1 Shock Tube

The classical shock tube problem, or Riemann problem, is commonly used to test numerical algorithms for hyperbolic conservation laws because it requires the resolution of all gas dynamic waves [46]. Consider a cylindrical tube with a thin membrane located at a known position with its surface oriented axially as shown by Fig. 3.3. The membrane separates an initially stagnant gas with a different thermodynamic state on each side. Quantities on the left and right sides of the membrane are denoted by “l” and “r” subscripts. Gas flow occurs once the membrane is ruptured, and a rarefaction, contact, and shock wave are observed. The analytical solution of this problem is determined from the conservation equations and the Rankine-Hugoniot relations which are valid across discontinuities [46].

The system of conservation laws that describes this flow are called the Euler equations of gas dynamics. These equations are given by Eqs. (2.4)-(2.6) with no cross-sectional area variations (i.e., \( \frac{dA}{dx} = 0 \)). The modeled domain was \( 0 \leq x \leq 1 \) m with the membrane located at
Figure 3.3: Schematic of the classical shock tube problem.

$x = 0.5$ m. Boundary conditions need not be imposed because the tube is sufficiently long such that the waves do not encounter the boundaries do not influence the flow. Also, the generalized coordinate transformation is not necessary since the physical domain is nondeforming (i.e., $\xi = \xi(x,t) = x$). All other parameters and initial conditions used for the simulation are summarized in Table 3.1.

Figure 3.4 shows the analytical solution and the predicted numerical results for the pressure, velocity, density, and temperature fields for $t = 0.6$ ms; the arrows in the figure indicate the direction of wave propagation. The contact and shock waves are discontinuous and travel from high to low pressure while the rarefaction wave is continuous and propagates in the opposite direction as the initially high gas pressure expands. The shock wave causes a jump in all four fields at approximately $x = 0.8$ m. The contact wave propagates more slowly than the shock and causes a jump in the density and temperature fields only. This wave is also called an entropy wave because it is associated with changes in entropy. The rarefaction wave travels in the opposite direction and spreads with time because the head of the wave travels faster than the tail of the wave.

Overall, the numerical results agree well with the exact solution. Typical of most high resolution techniques, some disagreement is observed near the contact wave where the numerical predictions are smeared. This disagreement is due to artificial viscosity, which is the inherent error in the numerical method. However, all wave speeds and the magnitude of the jumps are correctly predicted. The shock wave is captured in approximately 3-4 computational cells while the contact wave is captured in approximately 8-12 cells. Although not shown, the numerical results predicted by the LxF and NT techniques are much more smeared around the discontinuities and rarefaction tips due to artificial viscosity.
Table 3.1: Parameter values and initial conditions used for the classical shock tube problem.

<table>
<thead>
<tr>
<th>Parameter or Initial Condition</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
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<tr>
<td>$p_0^l$</td>
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<td>MPa</td>
</tr>
<tr>
<td>$p_0^r$</td>
<td>0.1</td>
<td>MPa</td>
</tr>
<tr>
<td>$R$</td>
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<td>J/(kg K)</td>
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<td>K</td>
</tr>
<tr>
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<td>250.0</td>
<td>K</td>
</tr>
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<td>m/s</td>
</tr>
<tr>
<td>$u_0^r$</td>
<td>0.0</td>
<td>m/s</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>1.4</td>
<td>—</td>
</tr>
<tr>
<td>$\theta$</td>
<td>1.25</td>
<td>—</td>
</tr>
</tbody>
</table>

Figure 3.4: Comparison of the analytical and numerical solutions for the classical shock tube problem at $t = 0.6$ ms: (a) pressure, (b) velocity, (c) density, and (d) temperature.
In order to establish the accuracy of the numerical method, a measure of numerical error must first be defined. Here, the numerical error at any given instance in time \( t^n \) is given by

\[
E(t^n) = \frac{1}{N_\xi} \sum_{j=1}^{N_\xi} \left| \frac{p(x_j, t^n) - \hat{p}(x_j, t^n)}{p^r} \right|,
\]

where \( p(x_j, t^n) \) is the numerically determined pressure at the spatial location \( x = x_j \), \( \hat{p}(x_j, t^n) \) is the analytical pressure at the same location, and \( p^r \) is a reference pressure used to nondimensionalize the equation [74]. The numerical error is evaluated such that the convergence rate, which gives the change in numerical error with grid resolution, can be determined. Assuming the error is proportional to the grid size raised to some power (i.e., \( E \propto \Delta x^\kappa \)), the resulting proportionality is obtained:

\[
\log \left( \frac{E}{p^r} \right) \propto \kappa \log (\Delta x),
\]

(3.20)

where \( \kappa \) is the convergence rate. Since the grid size is inversely proportional to the number of computational cells (i.e., \( \Delta x \propto 1/N_\xi \)), the following expression can be alternatively considered:

\[
\log \left( \frac{E}{p^r} \right) \propto \kappa \log \left( \frac{1}{N_\xi} \right),
\]

(3.21)

The convergence rate value is estimated by plotting \( \log(E) \) vs. \( \log(1/N_\xi) \) and fitting the data with a line of best fit. The slope of the line of best fit gives the convergence rate.

Figure 3.5 shows the convergence rate data for the shock tube problem. A range of \( 100 \leq N_\xi \leq 12800 \) computational cells were used in obtaining this data. The reference pressure was taken as the initial pressure on the left side of the membrane (i.e., \( p^r = p_0^l \)). The results indicate that the numerical error does indeed reduce as the grid is resolved at a rate of \( \kappa = 1.014 \). Although \( \kappa \approx 2 \) may be expected since the numerical method is nominally second-order accurate in space, high resolution shock capturing methods reduce to first-order accurate near discontinuities due to artificial viscosity.

### 3.3.2 Laval Nozzle

Another problem considered for numerical verification is steady flow through a Laval nozzle. Flow through Laval nozzles, also known as converging-diverging nozzles, is well understood because these types of nozzles are commonly used in jet and rocket engines. For steady sub-
sonic flow conditions upstream of the throat, there are three possible flow scenarios within the diverging section of the nozzle depending on back pressure, including 1) completely subsonic, 2) completely supersonic, and 3) transition from subsonic to supersonic with a stationary shock wave. If the flow leaving the nozzle is supersonic, corresponding to cases 2 and 3, the mass flow rate through the nozzle is choked and the Mach number is unity at the throat. For this analysis, completely subsonic and supersonic flow conditions through the diverging section of the nozzle are considered. The steady flow field is completely isentropic and the analytical solution is determined from the constant mass flow rate and isentropic relations [18].

Here, the shock tube problem with area variations is simulated until a steady flow field is obtained. Eqs. (2.4)-(2.6) are numerically solved on the fixed spatial domain $0 \leq x \leq 1$, and ghost nodes are incorporated at the non-reflecting boundary locations in order to allow incident waves to exit the domain. Again, the generalized coordinate transformation is not required since the physical space is nondeforming. The gas is initially stagnant and the membrane is located at the throat location $x = 0.5$ m. The prescribed cross-sectional area is $A(x) = \pi D(x)^2/4$ where the diameter is given by

$$D(x) = \begin{cases} 
D_l & \text{for } x \leq 0.25 \text{ m}, \\
\frac{(D_l + D_t)}{2} - \frac{(D_l - D_t) \cos (4\pi x)}{2} & \text{for } 0.25 \leq x \leq 0.50 \text{ m}, \\
\frac{(D_r + D_t)}{2} - \frac{(D_r - D_t) \cos (4\pi x)}{2} & \text{for } 0.50 \leq x \leq 0.75 \text{ m}, \\
D_r & \text{for } x \geq 0.75 \text{ m}. 
\end{cases}$$

(3.22)
The subscripts “l” and “r” denote the left and right sides of the throat which has diameter $D_t$. All other parameters and initial conditions used in the simulations are given in Table 3.2.

Table 3.2: Parameter values and initial conditions used for the Laval nozzle problem.

<table>
<thead>
<tr>
<th>Parameter or Initial Condition</th>
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<th>Value</th>
<th>Units</th>
<th>Supersonic Case</th>
<th>Value</th>
<th>Units</th>
</tr>
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</tr>
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<td>MPa</td>
</tr>
<tr>
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<td></td>
<td>0.1</td>
<td>MPa</td>
<td>$p_0^l$</td>
<td>0.1</td>
<td>MPa</td>
</tr>
<tr>
<td>$R$</td>
<td></td>
<td>287.0</td>
<td>J/(kg K)</td>
<td>$R$</td>
<td>287.0</td>
<td>J/(kg K)</td>
</tr>
<tr>
<td>$T_0^l$</td>
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<td>300.0</td>
<td>K</td>
<td>$T_0^l$</td>
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<td>K</td>
</tr>
<tr>
<td>$T_0^r$</td>
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<td>300.0</td>
<td>K</td>
<td>$T_0^r$</td>
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<td>K</td>
</tr>
<tr>
<td>$u_0^l$</td>
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<td>m/s</td>
<td>$u_0^l$</td>
<td>0.0</td>
<td>m/s</td>
</tr>
<tr>
<td>$u_0^r$</td>
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<td>0.0</td>
<td>m/s</td>
<td>$u_0^r$</td>
<td>0.0</td>
<td>m/s</td>
</tr>
<tr>
<td>$\gamma$</td>
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<td>1.5</td>
<td></td>
</tr>
</tbody>
</table>

The analytical solution and the numerical predictions are summarized in Fig. 3.6; the variation in radius of the nozzle with position is shown by the dashed line. In Fig. 3.6(a), the steady-state Mach number fields are shown for both cases considered. The Mach number increases in the converging section of the nozzle and remains constant where there are no area variations. In the subsonic case, the gas has a maximum Mach number of $Ma \approx 0.7$ at the throat. The gas then decelerates as the Mach number decreases in the diverging section of the nozzle due to the increasing cross-sectional area. On the other hand, the supersonic case reaches $Ma = 1.0$ at the throat then continues to increase in the diverging section of the nozzle. The ratio of static to stagnation pressure, density, and temperature are shown for the subsonic case in Fig. 3.6(b). All three thermodynamic properties decrease in the converging section of the nozzle as the gas expands then increase as the gas slows down and compresses in the diverging section. In the supersonic case, shown in Fig. 3.6(c), the thermodynamic properties decreases throughout the entire converging-diverging section as the gas expands. The numerical predictions in all three plots agree well with the analytical solutions across the entire domain.
Figure 3.6: Comparison of the analytical and numerical solutions for the Laval nozzle problem: (a) Mach number, and the thermodynamic property ratios for the completely (b) subsonic and (c) supersonic cases.

Figure 3.7 shows the convergence rate data for the case of complete supersonic flow through the diverging section of the nozzle. The numerical error was evaluated using Eq. (3.19) with the initial pressure on the left side of the throat used as the reference pressure (i.e., \( p^r = p^0_l \)), and a range of \( 100 \leq N_x \leq 12800 \) computational cells were used in obtaining the data. The numerical error reduces as the grid is resolved and at a rate of \( \kappa = 1.786 \). Here, the convergence rate is higher than the shock tube problem since the solution is continuous and differentiable across the domain (i.e., no shocks or rarefaction tips), but is slightly lower than \( \kappa = 2 \) due to the slope limiting procedure associated with the TVD property.
3.3.3 Retracting Pistons

For this problem, the grid metrics implementation is verified for a physical domain that distorts with time due to piston motion. As shown in Fig. 3.8, the problem consist of a tube with a constant cross-sectional area containing two pistons that confine an initially stagnant gas. As the pistons impulsively retract at constant velocities, rarefaction waves propagate from the pistons in the opposite direction of piston motion. Using conservation principles, a self-similar analytical solution can be formulated for each wave which holds before the waves meet and interact [75]. Because the physical domain stretches with time as the pistons retract, and the generalized coordinate transformation given by Eq. (3.4) is utilized. The governing conservation equations are again given by the Euler equations of gas dynamics without area variations (i.e., $\frac{dA}{dx} = 0$). The motion of the left and right boundaries are prescribed by

$$\frac{dx_{p,l}}{d\tau} = v_{p,l}, \quad \frac{dx_{p,r}}{d\tau} = v_{p,r},$$

(3.23)

where $x_{p,l}$ and $x_{p,r}$ are the piston boundary locations, $v_{p,l}$ and $v_{p,r}$ are the constant piston velocities, and the subscripts “$l$” and “$r$” denote left and right. The initial conditions of these equations are $x_{p,l}(0) = x_{p,l}^0$ and $x_{p,r}(0) = x_{p,r}^0$. A zero mass flux is imposed on the gas products at both boundaries which requires $u(x_{p,l}(t), t) = v_{p,l}$ and $u(x_{p,r}(t), t) = v_{p,r}$ for the entire simulation. The remaining initial conditions and parameters used in this study are summarized in Table 3.3.

Figure 3.7: Convergence rate plot for the Laval nozzle problem; supersonic flow case.
Table 3.3: Parameter values and initial conditions used for the retracting pistons problem.

<table>
<thead>
<tr>
<th>Parameter or Initial Condition</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
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<td>$R$</td>
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<td>J/(kg K)</td>
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<tr>
<td>$T^0$</td>
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<td>K</td>
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<tr>
<td>$u^0$</td>
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<td>m/s</td>
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</tr>
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<tr>
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<td>—</td>
</tr>
<tr>
<td>$\theta$</td>
<td>1.3</td>
<td>—</td>
</tr>
</tbody>
</table>

Figure 3.8: Schematic of the retracting pistons problem.

The analytical and numerical results for the velocity and pressure fields are shown at $t = 1.00$, 1.75, and 2.50 ms in Fig. 3.9; the left and right axis corresponds to the left and right piston locations at $t = 2.50$ ms, respectively. As shown by Fig. 3.9(a), the gas velocity behind each rarefaction wave is equal to its corresponding piston velocity while in front of each wave the gas remains stagnant. Also indicated by the figure, the gas undergoes larger expansion for faster traveling pistons which can be seen in the magnitude difference between the waves. Similar qualitative results are shown in the pressure fields of Fig. 3.9(b). Although some disagreement exist around the rarefaction tips due to artificial viscosity, the numerical predictions agree well with the analytical solutions in both plots. The wave speeds, magnitudes, and growth rates are accurately predicted by the model.

Figure 3.10 shows the convergence rate data based on the solution corresponding to $t = 1.75$ ms. The initial pressure was used as the reference pressure in Eq. (3.19), and a range
Figure 3.9: Comparison of the analytical and numerical solutions for the retracting pistons problem at $t = 1.00, 1.75, \text{ and } 2.50 \text{ ms}$: (a) velocity, and (b) pressure.

Figure 3.10: Convergence rate plot for the retracting pistons problem.

of $100 \leq N_\xi \leq 12800$ computational cells were used in obtaining the data. The convergence rate was calculated as $\kappa = 1.004$ which indicates that the numerical error reduces as the grid is resolved. Although there are no shocks or contact discontinuities in the solution, the first derivative of the solution is nonexistent at the rarefaction tips causing the reduced convergence rate.

Overall, good agreement exist between the exact analytical solutions and the numerical predictions for all three problems. Although the numerical predictions show slight disagreement around discontinuities and sharp edges, which is due to the inherent numerical error, the results are well resolved as compared to the LxF and NT techniques. The convergence
rate reduces to approximately $\kappa \approx 1$ for flow fields that have discontinuities in the solution or in the first derivative of the solution. This is a consequence of the shock capturing method. Although higher convergence rates could be achieved using a shock tracking method, these techniques require explicit tracking of discontinuities in the solution and are generally more complicated to implement. Nevertheless, the numerical model has good solution agreement and exhibits reasonable convergence rates for these three problems.
Chapter 4
Analysis of Explosively Actuated Nitrogen Cartridge Valves

In this chapter, predictions are presented and discussed for the explosively actuated nitrogen cartridge valve. In Section 4.1, predictions for the baseline valve configuration are first presented and the predictions are compared to available experimental data. The model’s sensitivity to parameters contained in the constitutive theory, and valve performance sensitivity to parameters of design importance are examined in Section 4.2. Lastly, predictions for geometrically similar, miniaturized valves are analyzed in Section 4.3.

4.1 Baseline Valve Predictions

All simulations for this study were performed on a Linux workstation having an INTEL Xeon 3.0 GHz processor with 4.6 Gb of memory. A typical run time for a single simulation having $N_\xi = 2000$ computational cells is approximately 30 minutes. This value of $N_\xi$ was used for all simulations performed in this study. Figure 4.1 gives the variation in predicted piston stroke time (discussed later) with increasing grid resolution for the baseline configuration; little variation exists for approximately $N_\xi > 1000$ nodes.

![Figure 4.1: Summary of the predicted variation in stroke time with spatial nodes for the baseline valve configuration.](image-url)
The baseline valve configuration is chosen to have dimensions that are representative of the conventional nitrogen cartridge valve shown in Figs. 1.1 and 1.2. The prescribed cross-sectional area variation of the baseline configuration is given by

\[ A(x) = D(x)^2 / 4, \]

where the diameter is

\[ D(x) = \begin{cases} 
D_a & \text{for } x \leq -L_e^0, \\
(D_a + D_t)/2 - (D_a - D_t) \cos (\pi x/L_e^0)/2 & \text{for } -L_e^0 \leq x \leq 0, \\
(D_{ec} + D_t)/2 - (D_{ec} - D_t) \cos (2\pi x/L_p^0)/2 & \text{for } 0 \leq x \leq L_p^0/2, \\
D_{ec} & \text{for } x \geq L_p^0/2.
\end{cases} \tag{4.1} \]

All other model parameters used in the baseline valve configuration are listed in Table 4.1.

<table>
<thead>
<tr>
<th>Parameter or Initial Cond.</th>
<th>Value</th>
<th>Units</th>
<th>Ref.</th>
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<th>Value</th>
<th>Units</th>
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Pressure field predictions for the baseline configuration are shown in Fig. 4.2 at various times following ignition; the horizontal arrows in the figures indicate the direction of wave propagation.
propagation, the dashed lines illustrate the axial variation in device radius; only the stretching
gas domain contained between the explosive and piston boundaries is shown. Immediately
following ignition at $t = 0$ $\mu$s, a product gas shock emanates from the explosive boundary
which strengthens as it propagates through the converging section of the device, driven by the
production of gas mass, momentum, and energy. This lead shock, as seen in Fig. 4.2(a) at
$t = 0.38$ $\mu$s, is partly transmitted through the port and into the expansion chamber causing
the gas mass flow rate to choke at the port throat. Some acoustic energy is reflected back
through the actuator further increasing the combustion rate as it subsequently interacts with
the explosive. Consequently, a secondary shock is formed near the explosive boundary that
again propagates toward the port. As these shocks propagate through the diverging section
of the expansion chamber, a compression wave develops behind the two shocks within the
expansion chamber, as seen in Fig. 4.2(a) at $t = 2.12$ $\mu$s. The subplot in Fig. 4.2(a) illustrates
these waves at $t = 2.12$ $\mu$s across the spatial domain $1.0 \leq x \leq 3.0$ mm. The compression
wave strengthens and becomes a third shock wave as it slowly follows the two leading shocks.
The first two shocks coalesce resulting in a single, stronger lead shock and multiple weak
rarefaction and contact waves. The new lead shock subsequently reflects off the piston surface
and coalesces with the third shock; again resulting in a single, stronger shock and multiple
weak rarefaction and contact waves. Though complex wave interactions occur within the
expansion chamber, the actuator pressure profiles remain smooth as combustion proceeds.
Figure 4.2(b) shows the pressure field at $t = 12.70$ $\mu$s, where a peak pressure of approximately
820 MPa is predicted within the actuator, and the remaining shock is observed at $x \approx 5.5$ mm.
As the actuator depressurizes, gas flow remains choked at the port. During this period,
pressure fields within the entire valve are mostly smooth with minimal wave interactions
occurring, as indicated in Fig. 4.2(b) at $t = 29.48$ $\mu$s. Figure 4.2(c) gives pressure field
predictions immediately after the shock passes through the port at $t = 41.37$ $\mu$s. At this time,
combustion is nearly complete and therefore largely unaffected by the impinging shock wave
that is subsequently reflected off the rear surface of the actuator located at $x \approx -2.3$ mm.
Pressure fields become complex after the shock passes through the port as indicated in Fig.
4.2(c) at $t = 57.40$ $\mu$s, and Fig. 4.2(d) at $t = 70.76$ $\mu$s. Complete combustion occurs at
$t_{barn} = 59.93$ $\mu$s, and the piston reaches its stroke at $t_{stk} = 93.74$ $\mu$s. Due to the abrupt stop
of the piston at stroke, a compression wave forms and propagates back through the expansion chamber as shown in Fig. 4.2(d) at $t = 95.30 \, \mu s$.

It is convenient and advantageous to analyze the temporal variation in average pressure within the actuator and expansion chamber. In this work, the volume average pressure is defined by

$$
\bar{p}(t) = \frac{1}{V(t)} \iiint p(x, t) \, dV,
$$

where $V(t)$ is the gas volume. The differential volume can be expressed as $dV = A(x)dx$ for the quasi-one-dimensional analysis, and the triple integral reduces to one in terms of $x$. Thus, the average actuator and expansion chamber gas pressures are given by
\[
\bar{p}_a(t) = \frac{1}{V_a(t)} \int_{-L_e(t)}^{0} p(x,t)A(x) \, dx, \quad (4.2)
\]

\[
\bar{p}_{ec}(t) = \frac{1}{V_{ec}(t)} \int_{0}^{L_p(t)} p(x,t)A(x) \, dx, \quad (4.3)
\]

where

\[
V_a(t) = \int_{-L_e(t)}^{0} A(x) \, dx, \quad V_{ec}(t) = \int_{0}^{L_p(t)} A(x) \, dx. \quad (4.4)
\]

The above integrals are evaluated numerically using the trapezoidal rule [37].

Figure 4.3(a) shows the variation in average actuator and expansion chamber pressure histories. The actuator rapidly pressurizes to a maximum value near 800 MPa at \( t \approx 12 \, \mu s \) due to the combined effects of explosive mass and energy release by combustion and choked flow through the port. The actuator pressure then decreases due to the increasing volume associated with the regressing explosive boundary while mass flow continues through the port and into the expansion chamber. The expansion chamber pressurizes more slowly than the actuator due to its larger volume and choked flow effects. The average pressures nearly equilibrate at \( t \approx 37 \, \mu s \), and both subsequently decrease due to volume increases with piston motion.

Figures 4.3(b) and (c) show the average, maximum, and minimum pressure histories within the actuator and expansion chamber, respectively. The maximum actuator pressure is taken as the largest pressure value at any spatial location within the actuator volume at a fixed instance in time; the minimum actuator and the expansion chamber maximum and minimum pressures are defined similarly. These figures are intended to highlight fluctuations about the mean due to gas dynamic waves within each volume; recall, the actuator gas volume extends from the explosive boundary to the port (i.e., \( L_e(t) \leq x \leq 0 \)) while the expansion chamber gas volume extends from the port to the piston face (i.e., \( 0 \leq x \leq L_p(t) \)). Until \( t \approx 40 \, \mu s \), few spatial fluctuations are observed in the actuator and the maximum actuator pressure remains close to the average value. The minimum actuator pressure is the pressure at the port during this time period and is significantly lower than the average due to large gas velocity and expansion. Similarly, as the expansion chamber pressurizes the maximum pressure is at the port location until \( t \approx 30 \, \mu s \), as seen in Fig. 4.3(c). The minimum expansion chamber pressure also deviates significantly from the average during this time due to shock wave interactions.
Figure 4.3: Predicted (a) spatially averaged gas pressure histories for the baseline valve. The maximum, minimum, and average gas pressure histories in the (b) actuator and (c) expansion chamber.

Once the remaining shock wave passes back through the port from the expansion chamber (see Figs. 4.2(b) and (c)), the location of the maximum and minimum pressures vary significantly due to complex gas dynamic pressure fields.

The predicted piston velocity and force histories for the baseline configuration are shown in Fig. 4.4. The piston velocity begins to increase only after the lead shock impinges upon it at $t \approx 6$ $\mu$s. Due to resistance and its inertia, the piston velocity smoothly increases to a maximum of 150 m/s at stroke despite the highly time-dependent pressure force acting on its boundary. The dynamic pressure force remains larger than the resistive force throughout the simulation resulting in a complex, but positive net force acting on the piston until stroke. Here,
the predicted resistive force is both qualitatively and quantitatively similar to that predicted by Braud, et al [14, 15].

Figure 4.5 shows the generated pyrotechnic shock for the baseline valve; the right hand axis gives the pyrotechnic shock in terms of g (i.e. $F_{pyro}(t) / m_d / 9.81$ m/s$^2$ where $m_d$ is the mass of the valve’s housing), and the sign corresponds to its direction of action. Initially, the pyrotechnic shock is dominated by the high gas pressure within the combustion zone. As combustion continues, the net strength of the pyrotechnic shock increases, and large oscillations are observed due to mechanical piston-housing interactions and gas dynamic pressure wave interactions with the device’s curved surfaces near the port. A maximum pyrotechnic force of approximately $-18$ kN ($-11,188$ g) at $t \approx 60$ µs is reached. Afterwords, the pyrotechnic shock decreases in magnitude with smaller oscillations until $t = t_{stk}$; during this time period, the average pressures decrease and the gas dynamic waves weaken due to the increasing device volume associated with piston motion down the bore. The instantaneous increase at $t = t_{stk}$ is due to the sudden piston impact against the piston stops which subsequently excites the gas dynamic fields. Large pyrotechnic shock oscillations are observed as gas waves propagate throughout the device, but they slowly decrease with time as the system equilibrates.
4.1.1 Zero Piston Resistance

A limiting case of zero piston resistance is now considered to establish the maximum velocity at stroke. Here, the piston resistance force is evaluated as $F_R = 0$ for all time while all other parameters and conditions are identical to the baseline case. The piston’s equation of motion, originally given by Eq. (2.21), reduces to

$$m_p \frac{d^2 (L_p)}{dt^2} = F_p.$$  \hspace{1cm} (4.5)

The gas dynamic fields are qualitatively similar to the baseline configuration, and the predicted complete combustion and stroke times are $t_{burn} = 63.09 \mu s$ and $t_{stk} = 75.16 \mu s$. Due to zero friction and no geometrical interference, the piston completes its stroke approximately 20 % faster than the baseline case. It does, however, take a slightly longer time period for complete combustion to occur. This is likely due to the faster expansion chamber volume increases which causes lower gas pressures throughout the valve.

The piston velocity and force histories are shown by Fig. 4.6. As seen in Fig. 4.6(a) for the case of zero resistance, the piston velocity quickly increases to a maximum value of 172 m/s at stroke, which is approximately 15 % greater than the baseline case. The piston force histories are shown in Fig. 4.6(b); recall, the net and pressure forces are equivalent for the case of
zero piston resistance. Without resistance, the net force closely replicates the baseline case pressure force until \( t \approx 25 \) \( \mu \)s. Differences occur thereafter due to rapid gas expansion from volume increases associated with piston motion. Nevertheless, the net force remains greater than that observed in the baseline case for most of the simulation resulting in a faster stroke time. In addition, the complex net force does not result in irregular or undesirable piston motion despite the lack of piston resistance. Therefore, piston inertia alone is sufficient to stabilize the piston against the dynamic pressure waves that act on the piston’s surface.

Figure 4.7(a) shows the average actuator and expansion chamber pressure histories. The expansion chamber pressures are indistinguishable until \( t \approx 25 \) \( \mu \)s. Due to fast piston motion, the expansion chamber volume increases more rapidly for the case of zero piston resistance and the average expansion chamber pressure decreases faster as a result. The rapid volume changes effect the actuator pressure in a similar manner, but not until the later time of \( t \approx 40 \) \( \mu \)s due to choked flow through the port.

Figure 4.7(b) shows the predicted pyrotechnic shock. The case of zero piston resistance exhibits similar qualitative trends as that observed in the baseline case. During most of the stroke time, however, the magnitude of the pyrotechnic shock is much larger for the case of zero piston resistance since the pyrotechnic shock component \( F_{ec}(t) = F_R(t) \) is zero during this time. In the baseline case, piston-housing interactions induce the resistive force which actually offset some of the loading induced by the large actuator pressure from combustion. A peak
force of approximately $-27$ kN ($-16,782$ g) at $t \approx 30$ μs is predicted which is approximately 50 % larger than the peak baseline value.

4.1.2 Experiment Comparisons

In the remainder of this section, the predicted average expansion chamber gas pressure and piston histories are compared to experimental results. The experiments were conducted at LANL using the gas gun system described earlier in Section 1.2 [24].

Gas pressure data were recorded by a pressure transducer located within the expansion chamber. Unfortunately, there is currently no experimental data available for the actuator due to the harsh environment created by the explosive combustion process. The pressure transducer was radially oriented near the port but outside the jet stream of gas. Figure 4.8(a) shows the experimentally measured and the predicted average expansion chamber pressure histories. The high frequency fluctuations in the experimental data are likely due to unwanted noise. Although the model over-predicts the magnitude, it does reasonably predict the pressurization rate and the low frequency oscillations observed after the peak pressure. The model predicts a maximum pressure of approximately 215 MPa while the experimental data indicates a maximum of approximately 170 MPa, both of which occur at $t \approx 40$ μs. The predictions for the case of zero piston resistance are also shown in the figure. After $t \approx 25$ μs, the case of zero piston resistance has better magnitude agreement with the experimental data, but does not exhibit the general depressurization trend since the expansion chamber volume quickly
Figure 4.8: Comparisons with experimental data: (a) spatially averaged expansion chamber pressure, and (b) piston velocity histories.

increases as explained in the previous section. Pressure differences between the model and the experimental results are possibly due to the model’s simplified valve geometry and the use of constant gas specific heats. Although it is unknown, this discrepancy is more likely due to incomplete combustion of the explosive in the experiment; lower pressures would be recorded if the explosive did not completely burn.

The experimental apparatus used to obtain piston velocity data closely replicated the nitrogen cartridge valve under consideration. In the experiments, the expansion chamber was replicated by a bore tube with similar geometrical features and material properties such that measurements could be made with VISAR. Since VISAR requires direct laser contact with the moving object, the piston is also exposed to atmospheric conditions in the experiment. Other key differences between the experimental apparatus and an actual valve include the lack of both piston stops and the nitrogen reservoir. However, the actuator and piston used in the experiments are identical to that used in an actual valve. Figure 4.8(b) shows the measured and predicted piston velocity histories. The fluctuations in the experimental data are possibly due to waves within the solid piston that are recorded by the highly sensitive VISAR. Overall, the model reasonably predicts the general trend and magnitudes as compared to the mean response of the experimental data. The case of zero piston resistance predicts much larger velocities as that observed in the experiments.
4.2 Parametric Analysis

In this section, model sensitivity to parameters imposed by the constitutive theory are first investigated, including the burn rate constants, number of explosive grains, and gas specific heats. Then, parameters that are important from a valve design perspective, including the port throat and explosive mass, are considered.

4.2.1 Model Parameters

4.2.1.1 Burn Rate Constants

The burn rate $r_e$ of solid energetics is commonly taken as pressure dependent and modeled by Eq. (2.16). The burn rate prefactor $a$ and exponent $n$ are usually obtained by closed bomb experiments. In this work, the baseline values of the burn rate parameters were taken from the literature for the explosive HMX [59]. A sensitivity analysis is conducted in this section to investigate model dependence on these burn rate parameters.

First, a range of burn rate exponents $0 \leq n \leq 0.86$ is considered where all other variables, including the burn rate prefactor, are fixed at their baseline values. Most explosives and propellants have values of $n$ that fall within this considered range [48, 59]. The predictions for this study are shown in Fig. 4.9 where the data is truncated after both the complete combustion and stroke times are reached. Figure 4.9(a) shows predicted histories for the mass fraction of burned explosive; this mass fraction is the ratio of solid explosive mass consumed by combustion over the initial solid explosive mass $m^0_e$, where the value $m^0_e = 1$ corresponds to complete combustion. The explosive burns rapidly for large values of $n$ with small variations in the predictions as compared to smaller values of $n$ which exhibit considerably slower burn rates. Figures 4.9(b) and (c) show the average actuator and expansion chamber pressure histories. The largest value of $n = 0.86$ exhibits fast actuator pressurization and a peak average pressure of approximately 1330 MPa, as seen in Fig. 4.9(b). Rapid combustion occurs with a predicted combustion and stroke time of $t_{burn} = 11.86 \mu s$ and $t_{stk} = 86.53 \mu s$ which are the fastest times for the range of $n$ considered. Lower peak actuator pressures and pressurization rates are observed for decreasing values of $n$, which causes lower burn rates and results in slower combustion and stroke times. For instance, complete combustion and stroke time predictions for the smallest case considered, $n = 0.70$, are $t_{burn} = 1183.61 \mu s$ and $t_{stk} = 436.36 \mu s$. As seen in Fig. 4.9(c), similar trends are observed in the average expansion chamber pressures...
with the exception of \( n \geq 0.84 \). Despite faster gas mass and energy release from combustion within the actuator, the predicted results are indistinguishable for \( n \geq 0.84 \) due to choked gas flow through the port which restricts expansion chamber pressurization. A summary of the predicted complete combustion and stroke times are shown in Fig. 4.9(d). As \( n \) increases, both the combustion and stroke times asymptotically approach minimum values. The combustion time approaches a minimum value of \( t_{\text{burn}} \approx 11 \mu s \) with increasing \( n \), and is more sensitive to changes in \( n \) as compared to the stroke time. The piston stroke time approaches a minimum value of \( t_{\text{stk}} \approx 87 \mu s \). The predicted baseline stroke time, \( t_{\text{stk}} = 93.74 \mu s \), is only approximately 8 \% greater than the minimum. In addition, the predicted stroke times for \( n \geq 0.79 \) are within 15 \% of the minimum value. Therefore, the predicted stroke times are largely insensitive to changes in burn rate exponent over this range, whereas considerable variations are observed for \( n < 0.79 \).

A range of burn rate prefactor \( 0.20 \times 10^{-7} \leq a \leq 8.00 \times 10^{-7} \text{ m/s Pa}^{-0.8} \) is now considered for fixed baseline variables including the burn rate exponent. This range of \( a \) considered is common for most explosives and propellants [48, 59]. The predicted results are qualitatively similar to the burn rate exponent analysis. Larger values of \( a \) yield rapid explosive combustion as indicated by the mass fraction of burned explosive histories in Fig. 4.10(a). Smaller values of \( a \) exhibit much slower burn rates with large variations in the predictions between cases. The average actuator and expansion chamber pressure histories are shown in Figs. 4.10(b) and (c). Peak average pressures of approximately 1275 and 225 MPa are predicted within the actuator and expansion chamber for the largest case considered, \( a = 8.00 \times 10^{-7} \text{ m/s Pa}^{-0.8} \). For decreasing values of \( a \), the burn rate decreases which results in lower peak pressures and pressurization rates within the actuator. The average expansion chamber pressures exhibit similar results with the exception of \( a \geq 6.00 \times 10^{-7} \text{ m/s Pa}^{-0.8} \). The predicted results are again indistinguishable within the expansion chamber for \( a \geq 6.00 \times 10^{-7} \text{ m/s Pa}^{-0.8} \) due to choked gas flow through the port, as explained earlier. Figure 4.10(d) shows a summary of the predicted complete combustion and stroke times; a logarithmic scale is used for the \( a \)-axis. The complete combustion and stroke times again asymptotically approach minimum values for increasing values of \( a \), with the combustion time exhibiting a greater sensitivity. The stroke time approaches \( t_{\text{stk}} \approx 87 \mu s \) with little variations in the predicted stroke times for
Figure 4.9: Predicted time histories for the burn rate exponent study: (a) mass fraction of burned explosive, average (b) actuator and (c) expansion chamber pressures. (d) Summary of the predicted variation in complete combustion and stroke times with burn rate exponent.

\[ a \geq 2.926 \times 10^{-7} \text{ m/s Pa}^{-0.8} \]; the predicted stroke times for this range of \( a \) are within 8 \% of the minimum approached value. Considerable variations are observed in piston stroke times for \( a < 2.926 \times 10^{-7} \text{ m/s Pa}^{-0.8} \).

4.2.1.2 Number of Explosive Grains

During combustion of a solid energetic, grains may fracture into smaller pieces due to the extreme environment, particularly right after ignition. This combustion behavior makes the number of explosive grains a difficult quantity to experimentally determine. In fact, this parameter contains the largest uncertainty in this work. The baseline value was chosen so that numerical predictions matched the pressure-time history obtained by firing the actuator into a 1 cc closed bomb [15]. Here, the influence of the number of burning grains on the model’s
predictions are investigated. All imposed parameters and conditions, including the explosive mass, are held fixed at their baseline values. Therefore, the size of the explosive grains (i.e. the grain radius $R_e$ and thus the burn surface area) must also vary in order to keep the explosive mass fixed and retain a physically meaningful analysis. For instance, the baseline number of explosive grains is $N_e = 10,000$ which corresponds to a grain radius of $R_e \approx 123 \, \mu m$. In this analysis, a range of $100 \leq N_e \leq 250,000$ is considered, which corresponds to a range in grain radius of approximately $572 \geq R_e \geq 42 \, \mu m$. Relative to the baseline value, the burn surface area is decreased by approximately 78.5 % for $N_e = 100$, and is increased by approximately 192.4 % for $N_e = 250,000$. 

Figure 4.10: Predicted time histories for the burn rate prefactor study: (a) mass fraction of burned explosive, average (b) actuator and (c) expansion chamber pressures. (d) Summary of the predicted variation in complete combustion and stroke times with burn rate prefactor.
Figure 4.11: Predicted time histories for the number of explosive grains study: (a) mass fraction of burned explosive, average (b) actuator and (c) expansion chamber pressures. (d) Summary of the predicted variation in complete combustion and stroke times with the number of explosive grains.

The predicted results are qualitatively similar to those for the burn rate constants given in the previous section. Figure 4.11(a) shows the time variation in mass fraction of burned explosive. Rapid combustion is observed for larger values of $N_e$ due to the increased burn surface area. The average actuator and expansion chamber pressure histories are shown in Figs. 4.11(b) and (c). Larger values of $N_e$ result in large peak pressures and pressurization rates as compared to the smaller values of $N_e$. The average expansion chamber pressure predictions are indistinguishable for $N_e \geq 100,000$. Figure 4.11(d) shows a summary of the predicted complete combustion and stroke times; the $N_e$-axis is a logarithmic scale. Again, the results asymptotically approach minimum values, and the combustion time exhibits greater
sensitivity to changes in $N_e$. The approached minimum stroke time is $t_{stk} \approx 87 \mu s$, and the predictions for $N_e \geq 5,000$ are within 15% of this value. On the other hand, the predicted stroke time is only sensitive to changes in the number of burning grains for $N_e < 5,000$.

4.2.1.3 Specific Heats

Model sensitivity to variations in gas specific heats, which are temperature dependent for ideal gases, are investigated in this section. The constant specific heats, and thus the specific heat ratio, used in the baseline configuration were estimated by the thermochemistry package CHEMKIN for $T = 3000$ K. Here, the considered specific heats are computed over the temperature range $300 \leq T \leq 8500$ K by the CHEMKIN subroutine library and database; a summary of the CHEMKIN analysis and results are given in Appendix A. The calculated specific heats with corresponding specific heat ratios are shown in Fig. 4.12 as a function of temperature. It should be noted, for fixed ideal gas constant $R$ and with $\gamma$ given, $c_p$ and $c_v$ are uniquely determined by $R = c_p - c_v$ and $\gamma = c_p/c_v$.

![Figure 4.12: Calculated specific heat data for the mixture of HMX combustion products.](image)

Figures 4.13(a) and (b) show the average actuator and expansion chamber pressure histories; each curve corresponds to a specific value of $\gamma$ for fixed $R$. Larger values of $\gamma$, corresponding to smaller specific heat values, exhibit large peak pressures and pressurization rates within both the actuator and expansion chamber. The predicted expansion chamber gas pressures
Figure 4.13: Predicted time histories for the specific heat study: average (a) actuator and (b) expansion chamber pressures. (c) Summary of the predicted variation in complete combustion and stroke times with the temperature at which the specific heats are evaluated.

for $\gamma \geq 1.295$ are much greater than that observed in the experimental data given in Section 4.1.2. Little variations are observed for $1.223 \leq \gamma \leq 1.250$ corresponding to the temperature range of $5500 \geq T \geq 2000$ K. The predicted complete combustion and stroke times are summarized in Fig. 4.13(c); the specific heat ratio is also shown on the right-hand axis as a reference. The results are largely insensitive to changes in specific heats over the temperature range of $2000 \leq T \leq 7000$ K. The predicted combustion and stroke times are within $\pm 6\%$ and $\pm 4\%$ of the baseline values over the insensitive temperature range. However, for $\gamma > 1.250$ corresponding to $T < 2000$ K and $T > 7000$ K, the predicted combustion and stroke times deviate significantly from the baseline values and exhibit a greater sensitivity.
4.2.2 Parameters of Design Importance

4.2.2.1 Port Diameter

The port diameter is varied in this analysis to investigate the effects of port cross-sectional area on valve performance. A range of valves are considered with port sizes that vary according to the port scale factor given by

\[ s_t = \frac{D_t}{D_t^*}, \]

where \( D_t^* \) denotes the baseline diameter given in Table 4.1; the baseline valve configuration is given by \( s_t = 1.0 \). A range of port scale factor \( 0.125 \leq s_t \leq 1.875 \) is considered in this study.

Figures 4.14(a) and (b) show the average actuator and expansion chamber pressure histories for several values of \( s_t \). As seen here, valves with small ports, corresponding to small values of \( s_t \), exhibit large peak pressures and pressurization rates within the actuator due to restricted gas flow into the expansion chamber and pressure enhanced combustion. Valves with larger ports, on the other hand, have much slower actuator pressurization due to the almost unobstructed gas transport through the port resulting in a slower burn rate. The fastest expansion chamber pressurization rate occurs for the baseline valve configuration where a peak pressure of approximately 215 MPa is predicted at \( t \approx 40 \mu s \). Small ports enable fast energy release of the explosive by promoting high actuator pressures, but are not capable of quickly transporting the energy through the smaller port cross-sectional areas. Although larger ports can accommodate fast energy transport, they cause low actuator pressurization and thus slow combustion energy release. Therefore, valves with either large or small port cross-sectional areas result in slow expansion chamber pressurization.

Figure 4.15(a) gives corresponding predictions for the piston velocity histories. The baseline valve configuration results in the fastest stroke time due to rapid expansion chamber pressurization. In addition to slow piston stroke times, valves with extreme values of \( s_t \) exhibit nonuniform piston velocity histories as compared to the baseline valve. For example, the valve corresponding to \( s_t = 0.125 \) exhibits an oscillatory behavior until \( t \approx 250 \mu s \) before rapidly increasing speed prior to stroke. Also, the valve corresponding to \( s_t = 1.875 \) exhibits slightly nonsmooth piston motion due to strong gas dynamic wave interactions at the piston.
surface. Although all cases considered result in successful valve operation, these extreme cases of $s_t$ exhibit irregular piston motion which is undesirable from a design perspective.

The predicted pyrotechnic shock for valves with port sizes corresponding to $s_t = 0.25, 1.0,$ and $1.875$ are shown in Fig. 4.15(b). High frequency oscillations are observed for $s_t = 0.25$ due to repeated energy reflections between the explosive boundary and the converging section of the port. In addition, this valve exhibits a relatively low pyrotechnic shock magnitude due to the large pressure force on the converging section of the port which offsets the opposing pressure force that acts on the actuator surface. As $s_t$ increases, fewer oscillations are observed while the magnitude of the pyrotechnic shock increases. A peak force of approximately $-26$ kN $(-16,161$ g) at $t \approx 105$ $\mu$s is reached for the extreme case of $s_t = 1.875$.

Figure 4.16 summarizes the predicted combustion and stroke times. Valves having $s_t < 1$ exhibit faster combustion times due to higher actuator pressurization rates induced by restricted gas flow through the smaller ports. Although the smaller ports result in higher combustion energy release rates, slower convective transport of this energy to the expansion chamber increases the stroke time. Valves having $s_t > 1$ enable greater convective energy transport to the expansion chamber, but reduce the combustion rate by limiting pressurization of the actuator. These predictions indicate that the baseline valve configuration results in optimal valve performance based on the piston stroke time.
Figure 4.15: Predicted (a) piston velocity and (b) pyrotechnic shock histories for the scaled port study.

Figure 4.16: Summary of the predicted variation in complete combustion and stroke times with port scale factor.

4.2.2.2 Explosive Mass

In this section, the amount of explosive mass is varied to determine its influence on valve performance. To this end, an explosive mass scale factor is defined by

\[ s_e \equiv \frac{m_e}{m_e^*}, \]

where \( m_e^* \) is the baseline value given in Table 4.1. The value of \( s_e \) is varied over the range \( 0.25 \leq s_e \leq 3.0 \), corresponding to \( 37.5 \leq m_e \leq 450.0 \) mg, in this analysis. The explosive grain
size (i.e., $R_e \approx 123 \, \mu m$) is held constant in the analysis while the number of explosive grains is varied to give the new desired mass. In addition, the initial clearance volume, defined here as the volume that extends from the initial explosive boundary to the port throat, is held constant throughout each case for consistency. The final actuator volume, however, varies according to the amount of solid explosive employed; the final axial length of the actuator varies and the diameter remains unchanged. Although two parameters are varied in this study (i.e., the amount of explosive mass and final actuator volume), this seems to be the most plausible way to change the amount of explosive mass used by the valve in practice.

Figures 4.17(a) and (b) show the average actuator and expansion chamber pressure histories. Valves with large values of $s_e$ exhibit large peak pressures and pressurization rates within both the actuator and expansion chamber due to the large output of explosive energy. The valve corresponding to $s_e = 3.0$ exhibits peak pressures of approximately 1580 MPa at $t \approx 13 \, \mu s$ in the actuator and 440 MPa at $t \approx 37 \, \mu s$ in the expansion chamber, respectively. As $s_e$ decreases, the peak pressures and pressurization rates decrease as well.

The piston velocity histories are shown in Fig. 4.18(a). The largest mass considered results in the fastest piston stroke time of $t_{stk} = 64.17 \, \mu s$ with a maximum piston velocity of 245 m/s at stroke. As $s_e$ decreases, and thus the available explosive energy release decreases, the piston stroke time increases and the piston velocity at stroke decreases. Valves corresponding to $s_e \leq 0.5$ exhibit irregular piston motion due to insufficient energy release. Furthermore,
Figure 4.18: Predicted (a) piston velocity and (b) pyrotechnic shock histories for the scaled explosive mass study.

The piston for the smallest explosive mass case did not successfully stroke resulting in valve failure.

Figure 4.18(b) shows the predicted pyrotechnic shock for $s_e = 0.375$, 1.0, and 3.0. Small magnitudes with few oscillations are predicted for small values of $s_e$. As $s_e$ increases, however, the maximum peak force of the pyrotechnic shock increases along with the amplitude of oscillations after the stroke time. The largest case considered exhibits the most detrimental pyrotechnic shock with a peak force of approximately $-48$ kN ($-29,835$ g) at $t \approx 51$ µs and large amplitude oscillations after piston stroke.

Figure 4.19 summarizes complete combustion and stroke times, both of which asymptotically approach minimum values for increasing $s_e$. Valves having small values of $s_e$ exhibit slow combustion and stroke times due to lower actuator and expansion chamber pressurization rates induced by the smaller explosive mass. Faster combustion and stroke times with smooth piston motion are predicted for valves with large values of $s_e$, but at the cost of larger pyrotechnic shocks. Only a marginal gain in stroke time is obtained, with a large increase in pyrotechnic shock, for $s_e > 2$. These predictions indicate a sensitivity to explosive mass that must be considered in valve design.

There exist other system parameters that may influence valve performance, including the piston mass, the device cross-sectional area profile, etc. Figure 4.20(a) illustrates the gas pressure field predictions at $t = 1.45$ and $t = 4.62$ µs obtained by increasing the clearance.
Figure 4.19: Summary of the predicted variation in complete combustion and stroke times with explosive mass scale factor.

volume by approximately 140% relative to the baseline value. To this end, the initial explosive boundary is placed at $L_e^0 = 1.338$ mm; with all other system parameters fixed at their baseline values, including the prescribed actuator cross-sectional area variations. Unlike the baseline predictions which indicate mostly smooth spatial variations in actuator pressure, non-uniform variations are now predicted due to stronger wave reflections occurring between the explosive boundary and the converging section of the port. These wave reflections induce less uniform explosive combustion. Figure 4.20(b) compares the predicted product gas mass flow rate through the boundary (i.e., $\dot{m}_g$) to that of the baseline configuration. The combustion rate is also less than the baseline configuration due lower pressure within the larger clearance volume. Despite stronger wave interactions, the predicted piston motion remains smooth and uniform.

The complete combustion and stroke times occur at $t_{\text{burn}} = 71.68$ $\mu$s and $t_{\text{stk}} = 105.37$ $\mu$s, respectively, which are larger than those of the baseline valve due to slower combustion energy release. Qualitatively similar results are obtained for variations in actuator geometry, as shown in Fig. 4.21 for an actuator diameter variation given by

$$D(x) = \begin{cases} 
D_a & \text{for } x \leq -L_e^0/2, \\
(D_a + D_t)/2 - (D_a - D_t) \cos \left( \frac{2\pi x}{L_e^0} \right) / 2 & \text{for } -L_e^0/2 \leq x \leq 0,
\end{cases}$$

(4.6)

where the actuator diameter is increased to $D_a = 6.712$ mm.
4.3 Miniature Explosive Valves

The goal of the study presented in this section is to examine how the predicted performance of the baseline explosively actuated valve varies with a linear reduction in size. All of the miniaturized valves considered are geometrically similar with dimensions that are reduced by a uniform scale factor defined by

$$s = \frac{l}{L}.$$ 

The baseline valve configuration discussed in Section 4.1 corresponds to $s = 1.0$. For a baseline
dimension of $L$, the miniaturized valve has a corresponding linearly reduced dimension given by $l$. A range of valves with geometrical scale factor $0.125 \leq s \leq 1.0$ are considered in this study. As done for the explosive mass study, the explosive grain size is fixed at the baseline value while the number of grains is reduced according to the scaled actuator volume. All other parameters are fixed at their baseline value, including all piston-housing material properties and explosive burn properties. In addition, the effects associated with scale-dependent surface tribology and thermomechanical material properties are not accounted for in this analysis. Therefore, the predicted results only give leading order estimates for the variation in valve operation and performance with size.

In this work, the valves are categorized in a similar manner to that first proposed by Gonthier, et al [33]. Three classes of valves are identified based on the mass specific piston kinetic energy at stroke and the piston velocity histories: overdriven, transitional, and underdriven. Figure 4.22 shows the variation in both mass specific piston kinetic energy at stroke and piston mass with geometric scale factor, and Figs. 4.23(a) and (b) show the predicted piston position and velocity histories for different scale factors. Overdriven valves have stroke velocities, and thus mass specific kinetic energies, that are largely insensitive to geometric scale. These valves range from $0.75 \leq s \leq 1.0$ and have piston position and velocity histories that monotonically increase with time until stroke. Predicted stroke times range from $t_{stk} = 93.74 \mu s$ for $s = 1.0$ to $75.77 \mu s$ for $s = 0.75$, corresponding to stroke lengths of 6.0 mm and 4.5 mm. Piston velocity histories for underdriven valves, corresponding to $0.125 \leq s \leq 0.4375$, indicate a sensitivity to geometric scale, and are less monotonic resulting in irregular piston motion. For example, the piston velocity of the valve corresponding to $s = 0.3125$ quickly increases initially, but then slowly accelerates for approximately $20 \leq t \leq 30 \mu s$ before quickly increasing again to a final velocity of approximately 115 m/s at the stroke time $t_{stk} = 62.75 \mu s$. In fact, underdriven valves corresponding to $0.23 < s < 0.30$ have piston velocity histories with a period of deceleration, as seen in Fig. 4.23(b) for the valve corresponding to $s = 0.25$ during approximately $20 \leq t \leq 30 \mu s$. This range of underdriven valves exhibit slightly larger stroke velocities due to larger expansion chamber pressures induced by the piston deceleration period; this is illustrated by the local maximum near $s = 0.27$ in Fig. 4.22. Although the piston reaches the stops for all underdriven valves considered, the predicted piston motion his-
Figure 4.22: Summary of the predicted variation in mass specific piston kinetic energy at stroke with geometric scale factor.

Figure 4.23: Predicted piston (a) position and (b) velocity histories for geometrically scaled valves.

Stories indicate that irregular behavior may result in practice for valves of this geometrical size and configuration. Transitional valves border underdriven valve behavior and give a practical design limit for the miniature valves.

Figures 4.24(a) and (b) show the average actuator and expansion chamber pressure histories; the results are truncated after the stroke time for clarity. Peak average actuator pressures decrease significantly with geometric scale factor. Overdriven valves attain peak actuator pressures of $615 \leq \overline{p_a} \leq 800$ MPa before depressurizing due to gas flow through the port into the expansion chamber; peak expansion chamber pressures are in the range $200 \leq \overline{p_{ec}} \leq 215$ MPa.
Figure 4.24: Predicted average (a) actuator and (b) expansion chamber pressure histories for geometrically scaled valves.

It is desirable to have large pressurization within both the actuator and expansion chamber for rapid combustion and monotonically increasing piston motion. Underdriven valves exhibit low actuator pressurization rates caused by the combined effects of smaller explosive burn surface area and fast flow of gas mass through the port relative to the combustion rate. Lower expansion chamber pressurization rates are therefore observed in underdriven valves due to the slower combustion rates. In addition, the predicted peak expansion chamber pressures for underdriven valves are sensitive to geometric scale. For example, valves that have predicted piston deceleration periods, corresponding to $0.23 < s < 0.30$, have slightly larger peak expansion chamber pressures due to the slower gas volume expansion rates.

The predicted pyrotechnic shock for $s = 1.0, 0.5, 0.25,$ and $0.125$ are shown by Figs. 4.25(a)-(d). As the valves reduce in size, the predicted pyrotechnic shock exhibits larger amplitudes with higher frequencies due to gas dynamic interactions. As seen in Fig. 4.25(d), the smallest valve considered has the most detrimental pyrotechnic shock with a peak magnitude of approximately $50,500 \text{ g}$ at $t \approx 84 \mu s$, and an amplitude of approximately $\pm 20,000 \text{ g}$ after the stroke time.

Figure 4.26 summarizes the predicted variation in complete combustion and stroke time with geometric scale factor. Overdriven valves are characterized by complete or nearly complete explosive combustion prior to piston stroke, while underdriven valves are characterized by much slower combustion times relative to stroke time.
Figure 4.25: Predicted pyrotechnic shock histories for geometrically scaled valves corresponding to (a) $s = 1.0$, (b) 0.5, (c) 0.25, and (d) 0.125.
Figure 4.26: Summary of the predicted variation in complete combustion and stroke times with geometric scale factor.
Chapter 5
Conclusions

The primary objective of this thesis was to develop a mathematical model for explosively actuated devices that can be used to examine the effect of design modifications on device performance and on the produced pyrotechnic shock. The model includes a gas dynamic analysis with the following features: 1) acoustic mass and energy transport within and between the actuator and expansion chamber, 2) gas dynamic wave interactions with both the combustion process and piston motion, 3) piston dynamics coupled with device elastic-plastic deformation, 4) device cross-sectional area variations, and 5) gas volume changes due to solid explosive combustion and piston motion.

The model was posed as a mathematical IBVP which was solved numerically in generalized coordinates using a TVD, high resolution shock capturing method. A numerical verification study composed of three problems was conducted in order to verify the numerical algorithm and gain confidence in the model’s predictions. The numerical results had good agreement with the analytical solutions and exhibited reasonable convergence rates for all three problems.

Predictions for the baseline valve configuration agree reasonably well with experimental data for piston stroke time (i.e., \( t \approx 90 \, \mu s \)), expansion chamber pressurization rate, and piston velocity; the model over predicts the magnitude of the expansion chamber pressure which is possibly due to incomplete combustion. Though complex pressure fields were predicted in the expansion chamber, baseline valve predictions indicate that piston motion is largely insensitive to the gas dynamic pressure force acting on its surface due to piston resistance and inertia. In fact, piston inertia alone is sufficient to stabilize the piston against gas dynamic pressure wave interactions as seen in the limiting case of zero piston resistance analysis. Also, the combustion process is largely unaffected by gas dynamics waves due to choked gas flow through the port. The predictions indicate that gas dynamic wave interactions do not significantly effect valve performance for the considered nitrogen cartridge valve.

Two valve parameters, namely port cross-sectional area and explosive mass, were investigated to identify their effects on valve performance. It was demonstrated that port size controls both combustion energy release and convective energy transport through the port
which effects piston motion and valve operation time. Valves with large ports exhibited slow combustion energy release while valves with small ports exhibited slow energy transport to the expansion chamber. For this study, the baseline valve configuration resulted in optimal valve performance based on stroke time. It was also demonstrated how the amount of explosive mass effects both valve performance and the pyrotechnic shock. Valves with too little explosive mass result in irregular piston motion and slow valve operation time. However, too much explosive results in large pyrotechnic shock loading with only a small improvement in valve operation time. An optimal amount of explosive mass was not identified in this study due to the adverse effects of pyrotechnic shock loading. Clearly, a valve performance sensitivity to both the port size and amount of explosive mass were identified that must be considered in valve design.

Variations in performance of miniature explosive valves (i.e., the baseline configuration with a linear reduction in size) were also examined in this work. The analysis identified three performance levels that depend on scale $s$ ($0 < s \leq 1.0$, where $s = 1.0$ is the baseline configuration) corresponding to overdriven, transitional, and underdriven valves. Optimal valve performance, as demonstrated by mildly overdriven valves, results from both rapid combustion and expansion chamber pressurization rates. Overdriven valves ($0.75 \leq s \leq 1.0$) perform successfully with smooth, monotonic increases in piston velocity throughout its stroke. Underdriven valves ($0.125 \leq s \leq 0.4375$) result in irregular, oscillatory piston motion that is undesirable from a design perspective. This undesirable behavior is largely the manifestation of coupled interactions between pressure-dependent explosive combustion within the actuator, and compressible flow of combustion product gases through the port and into the expansion chamber, both of which limit the expansion chamber pressurization rate.

There are several improvements that could be made to the model in order to better resemble explosively actuated devices. It is recommended to improve the solid explosive combustion model and include a burst disc at the port. Although the current combustion model accounts for pressure-dependent burn of multiple explosive grains with spherical geometry, all of the burning grains are assumed to burn at the same rate and in an unlikely organized manner within the actuator (i.e., contained within the combustion zone). It is suggested to include two-phase (reactive solid and inert gas) flow within the valve based on the well-established continuum mixture model of Baer and Nunziato [1] which was later improved by Bdzil, et
al [4], and Kapila, et al [36]. By incorporating a two-phase flow description, the combustion model could accommodate nonuniform explosive burning and eliminate the movable explosive boundary. In addition, solid explosive transport and combustion within the expansion chamber could be addressed. It is also suggested to include the burst disc in the model. The burst disc will likely effect the combustion process and possibly cause stronger lead shocks within the expansion chamber that are sufficient to drive the piston to stroke. Both of these suggestions would result in a more accurate model that better represents explosively actuated devices.
References


Appendix A
Summary of the CHEMKIN Analysis

The commercially available software package CHEMKIN was utilized in obtaining the HMX combustion product gas constant and specific heats. A summary of the CHEMKIN analysis is presented in this appendix.

An equilibrium chemistry calculation was performed using CHEMKIN to determine the gas products produced from solid HMX \((C_4H_8N_8O_8)\) combustion. The analysis imposed constant internal energy and constant volume. The resulting stoichiometric equation for the combustion of solid HMX is shown in Table A.1. Similar results were obtained by Tarver, et al [71], for finite rate HMX combustion.

In this study, the gas is modeled as a single species with properties of the combustion product gas mixture (i.e., HMX (s) \(\rightarrow\) HMX product (g)). The calculated molecular weight of the gas composition given above was \(\bar{m} = 24.629\) kg/kmol yielding an ideal gas constant of \(R = 337.590\) J/(kg K). The specific heats were calculated over a range of temperatures for fixed gas composition using the CHEMKIN subroutine library and database. The calculated specific heats at constant volume \(c_v\) and pressure \(c_p\), along with the corresponding specific heat ratios \(\gamma\), are given in Table A.2 and plotted in Fig. A.1 as a function of temperature. Specific heats \(c_v = 1436.58\) and \(c_p = 1774.17\) J/(kg K) corresponding to \(\gamma = 1.235\) at \(T = 3000\) K were chosen for the baseline valve configuration.

Table A.1: HMX chemical combustion equation.

<table>
<thead>
<tr>
<th>(C_4H_8N_8O_8(s))</th>
<th>(\rightarrow)</th>
<th>3.979 N(_2)(g) + 2.971 CO(g) + 2.908 H(_2)O(g) + 1.005 CO(_2)(g)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>+ 0.999 H(_2)(g) + 0.062 OH(g) + 0.035 H(g) + 0.002 NO(g)</td>
</tr>
</tbody>
</table>
Table A.2: Specific heat data for the mixture of HMX combustion products.

<table>
<thead>
<tr>
<th>Temperature $T$, (K)</th>
<th>Specific Heat Data</th>
<th>Specific Heat Ratio, $\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$c_v$, (J/kg/K)</td>
<td>$c_p$, (J/kg/K)</td>
</tr>
<tr>
<td>300</td>
<td>912.80</td>
<td>1250.40</td>
</tr>
<tr>
<td>500</td>
<td>972.79</td>
<td>1310.39</td>
</tr>
<tr>
<td>1000</td>
<td>1144.91</td>
<td>1482.51</td>
</tr>
<tr>
<td>1500</td>
<td>1270.29</td>
<td>1607.89</td>
</tr>
<tr>
<td>2000</td>
<td>1351.14</td>
<td>1688.74</td>
</tr>
<tr>
<td>2500</td>
<td>1402.65</td>
<td>1740.25</td>
</tr>
<tr>
<td>3000</td>
<td>1436.58</td>
<td>1774.17</td>
</tr>
<tr>
<td>3500</td>
<td>1461.23</td>
<td>1798.83</td>
</tr>
<tr>
<td>4000</td>
<td>1481.50</td>
<td>1819.10</td>
</tr>
<tr>
<td>4500</td>
<td>1498.81</td>
<td>1836.41</td>
</tr>
<tr>
<td>5000</td>
<td>1511.17</td>
<td>1848.76</td>
</tr>
<tr>
<td>5500</td>
<td>1513.13</td>
<td>1850.73</td>
</tr>
<tr>
<td>6000</td>
<td>1495.82</td>
<td>1833.42</td>
</tr>
<tr>
<td>6500</td>
<td>1446.93</td>
<td>1784.53</td>
</tr>
<tr>
<td>7000</td>
<td>1350.70</td>
<td>1688.29</td>
</tr>
<tr>
<td>7500</td>
<td>1187.93</td>
<td>1525.52</td>
</tr>
<tr>
<td>8000</td>
<td>935.99</td>
<td>1272.59</td>
</tr>
<tr>
<td>8500</td>
<td>568.82</td>
<td>906.42</td>
</tr>
</tbody>
</table>

Figure A.1: Calculated specific heat data for the mixture of HMX combustion products.
Appendix B
Derivation of the Net Axial Pressure Force

The net axial pressure force that acts on the curved surface of the valve and contributes to the pyrotechnic shock is derived in this appendix.

Consider a cross-sectional slice of the valve with thickness $dx$ as shown in Fig. B.1. For an infinitely thin section (i.e., $dx \to 0$), the curvature approaches a straight line such that the geometry of the section exhibits a conical frustum. The local pressure force that acts normal to this section is given by

$$f_{p,N}(x,t) = p(x,t) A_l(x)$$ (B.1)

where $A_l(x)$ is the lateral surface area of the frustum as indicated by the shaded region in Fig. B.1. Based on the geometry, this surface area is evaluated by

$$A_l(x) = 2 \pi R(x) l,$$

$$= 2 \pi R(x) \frac{dx}{\sin \alpha}. \quad \text{(B.2)}$$

Therefore, the local axial pressure force is given by

$$f_{p,a}(x,t) = f_{p,N}(x,t) \cos \alpha,$$

$$= p(x,t) 2 \pi R(x) \frac{dx}{\sin \alpha} \cos \alpha,$$

$$= p(x,t) 2 \pi R(x) \frac{dx}{\tan \alpha}.$$ \quad \text{(B.3)}

Using the slope of the profile $\frac{dR}{dx}$, the angle $\alpha \in [0, \pi/2]$ is evaluated by

$$\tan \alpha = - \frac{1}{\frac{dR}{dx}}, \quad \text{(B.4)}$$

where the negative sign is needed since the slope is negative for the section under consideration. Substituting back into Eq. (B.3) and rearranging terms results in

$$f_{p,a}(x,t) = -2 \pi p(x,t) R(x) \frac{dR}{dx} dx.$$ \quad \text{(B.5)}
Notice for the curved surface of the actuator (i.e., $x \leq 0$), the derivative of $R(x)$ is negative and Eq. (B.5) is positive. Therefore, the local axial pressure force at that location is in the correct, positive direction. On the other hand, the derivative of $R(x)$ is positive for the curved surface of the expansion chamber (i.e., $x \geq 0$), and the local axial pressure force acts on the valve housing in the negative direction as it should. The net axial pressure force is found by integrating Eq. (B.5):

$$F_{p,a}(t) = -2\pi \int_{L_e(t)}^{L_p(t)} p(x,t) R(x) \frac{dR}{dx} dx.$$  

(B.6)

By substituting $R(x) = D(x)/2$, Eq. (2.31) is recovered:

$$F_{p,a}(t) = -\frac{\pi}{2} \int_{L_e(t)}^{L_p(t)} p(x,t) D(x) \frac{dD}{dx} dx.$$  

(B.7)

For portions of the valve without curvature, the derivative of $D(x)$ is zero and no contribution is made to the axial pressure force.
Figure B.1: Schematic used in deriving the net axial pressure force component of the pyrotechnic shock.
Appendix C
Derivation of the Generalized Coordinate Transformation

An expression for the grid metrics, transformed model equations in terms of the fixed computational coordinates \((\xi, \tau)\), and the eigenvalues of the generalized flux Jacobian are derived in this appendix.

The governing equations in terms of the physical coordinate system are given by Eqs. (2.4)-(2.6), and are written in vector conservative form as

\[
\frac{\partial}{\partial t} \hat{q}(x,t) + \frac{\partial}{\partial x} \hat{f}(x,t) = \hat{w}(x,t),
\]

where \( \hat{q}, \hat{f}, \) and \( \hat{w} \) are the conserved, nonlinear flux, and source vectors given by

\[
\hat{q} = [\rho, \rho u, \rho E]^T,
\]
\[
\hat{f} = \left[ \rho u, \rho u^2 + p, \rho u \left( E + \frac{p}{\rho} \right) \right]^T,
\]
\[
\hat{w} = \left[ -\rho u \frac{1}{A} \frac{\partial A}{\partial x}, -\rho u^2 \frac{1}{A} \frac{\partial A}{\partial x}, -\rho u \left( E + \frac{p}{\rho} \right) \frac{1}{A} \frac{\partial A}{\partial x} \right]^T.
\]

Equation (C.1) is transformed to the generalized computational space by taking

\[
\xi = \xi(x,t), \quad \tau = \tau(x,t) = t,
\]

where time is a direct transformation since time is equivalent in both domains. Using the chain rule, partial derivatives are expressed as

\[
\left. \frac{\partial}{\partial x} \right|_t = \xi_x |_t \left. \frac{\partial}{\partial \xi} \right|_\tau, \quad \left. \frac{\partial}{\partial t} \right|_x = \xi_t |_x \left. \frac{\partial}{\partial \xi} \right|_\tau + \left. \frac{\partial}{\partial \tau} \right|_\xi,
\]

where \( \xi_t \) and \( \xi_x \) are the grid metrics. Expressions for the metrics are derived by considering differential changes in each coordinate system. Changes in the generalized coordinates can be written as

\[
d\xi = \xi_x \, dx + \xi_t \, dt, \quad d\tau = dt,
\]

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or in matrix form:

\[
\begin{bmatrix}
  d\xi \\
  d\tau
\end{bmatrix} =
\begin{bmatrix}
  \xi_x & \xi_t \\
  0 & 1
\end{bmatrix}
\begin{bmatrix}
  dx \\
  dt
\end{bmatrix}.
\] (C.5)

Assuming Eq. (C.2) can be inverted such that the relations \( x = x(\xi, \tau) \) and \( t = \tau \) exist, changes in the physical coordinates can be written as

\[
dx = x_\xi d\xi + x_\tau d\tau, \quad dt = d\tau,
\] (C.6)

or in matrix form:

\[
\begin{bmatrix}
  dx \\
  dt
\end{bmatrix} =
\begin{bmatrix}
  x_\xi & x_\tau \\
  0 & 1
\end{bmatrix}
\begin{bmatrix}
  d\xi \\
  d\tau
\end{bmatrix}.
\] (C.7)

Solving for \( d\xi \) and \( d\tau \) in Eq. (C.7) gives

\[
\begin{bmatrix}
  d\xi \\
  d\tau
\end{bmatrix} =
\begin{bmatrix}
  x_\xi & x_\tau \\
  0 & 1
\end{bmatrix}^{-1}
\begin{bmatrix}
  dx \\
  dt
\end{bmatrix}.
\] (C.8)

By comparing Eqs. (C.5) and (C.8), the following matrix relation must hold:

\[
\begin{bmatrix}
  \xi_x & \xi_t \\
  0 & 1
\end{bmatrix} =
\begin{bmatrix}
  x_\xi & x_\tau \\
  0 & 1
\end{bmatrix}^{-1}.
\] (C.9)

Using the method of cofactors, the matrix on the right hand side of Eq. (C.9) above becomes

\[
\begin{bmatrix}
  x_\xi & x_\tau \\
  0 & 1
\end{bmatrix}^{-1} = \frac{1}{x_\xi}
\begin{bmatrix}
  1 & -x_\tau \\
  0 & x_\xi
\end{bmatrix},
\]

\[
= \begin{bmatrix}
  1/x_\xi & -x_\tau/x_\xi \\
  0 & 1
\end{bmatrix}.
\] (C.10)

Thus, the grid metrics are found by substituting Eq. (C.10) into (C.9) resulting in

\[
\xi_x = \frac{1}{x_\xi} = J, \quad \xi_t = \frac{x_\tau}{x_\xi},
\] (C.11)
which is identical to that presented in Section 3.1 (i.e., Eq. (3.7)). Again, $\xi_x$ is the Jacobian that accounts for spatial deformation.

With the grid metrics known, the governing equations are now transformed into the generalized computational space. Applying Eq. (C.3) to (C.1) results in

$$\frac{\partial \hat{q}}{\partial \tau} + \xi_t \frac{\partial \hat{q}}{\partial \xi} + \xi_x \frac{\partial \hat{f}}{\partial \xi} = \hat{w}. \quad (C.12)$$

In order to apply the KT numerical technique, the governing equations must be expressed in conservative form. Using the grid metric expressions given by Eq. (C.11), Eq. (C.12) becomes

$$\frac{\partial \hat{q}}{\partial \tau} - \frac{x_r}{x_\xi} \frac{\partial \hat{q}}{\partial \xi} + \frac{1}{x_\xi} \frac{\partial \hat{f}}{\partial \xi} = \hat{w},$$

$$\frac{\partial \hat{q}}{\partial \tau} - x_r J \frac{\partial \hat{q}}{\partial \xi} + J \frac{\partial \hat{f}}{\partial \xi} = \hat{w}. \quad (C.13)$$

Dividing through by $J$ gives

$$\frac{1}{J} \frac{\partial \hat{q}}{\partial \tau} - \frac{x_r}{x_\xi} \frac{\partial \hat{q}}{\partial \xi} + \frac{1}{J} \frac{\partial \hat{f}}{\partial \xi} = \frac{\hat{w}}{J}. \quad (C.14)$$

Substituting the relations

$$\frac{\partial}{\partial \tau} \left( \frac{\hat{q}}{J} \right) = \frac{1}{J} \frac{\partial \hat{q}}{\partial \tau} + \hat{q} \frac{\partial}{\partial \tau} \left( \frac{1}{J} \right),$$

$$= \frac{1}{J} \frac{\partial \hat{q}}{\partial \tau} + \hat{q} x_r \xi,$$

$$\Rightarrow \frac{1}{J} \frac{\partial \hat{q}}{\partial \tau} = \frac{\partial}{\partial \tau} \left( \frac{\hat{q}}{J} \right) - \hat{q} x_r \xi,$$

and

$$\frac{\partial}{\partial \xi} \left[ -x_r \hat{q} + \hat{f} \right] = -x_r \frac{\partial \hat{q}}{\partial \xi} - x_r \xi \hat{q} + \frac{\partial \hat{f}}{\partial \xi},$$

$$\Rightarrow -x_r \frac{\partial \hat{q}}{\partial \xi} + \frac{\partial \hat{f}}{\partial \xi} = \frac{\partial}{\partial \xi} \left[ -x_r \hat{q} + \hat{f} \right] + x_r \xi \hat{q},$$

into Eq. (C.14) and rearranging terms results in

$$\frac{\partial}{\partial \tau} \left( \frac{\hat{q}}{J} \right) + \frac{\partial}{\partial \xi} \left[ -x_r \hat{q} + \hat{f} \right] = \frac{\hat{w}}{J}. \quad (C.15)$$
Again using the derived expressions for the grid metrics, Eq. (C.15) is expressed as

\[
\frac{\partial}{\partial \tau} \left( \mathbf{q} \right) + \frac{\partial}{\partial \xi} \left[ \xi \mathbf{q} + \xi_x \mathbf{f} \right] = \mathbf{w}.
\]

(C.16)

Finally, the governing conservation equations in generalized conservative form is

\[
\frac{\partial \mathbf{q}}{\partial \tau} + \frac{\partial \mathbf{f}}{\partial \xi} = \mathbf{w},
\]

(C.17)

where \( \mathbf{q}, \mathbf{f}, \) and \( \mathbf{w} \) are the conserved, nonlinear flux, and source vectors expressed in generalized coordinates given by

\[
\mathbf{q} = \frac{\mathbf{\hat{q}}}{J} = \left[ \frac{\rho}{J}, \frac{\rho u}{J}, \frac{\rho E}{J} \right]^T,
\]

\[
\mathbf{f} = \frac{\xi \mathbf{\hat{q}} + \xi_x \mathbf{\hat{f}}}{J} = \left[ \frac{\rho U^c}{J}, \frac{\rho u U^c + \xi_x p}{J}, \frac{\rho E U^c + \xi_x u p}{J} \right]^T,
\]

\[
\mathbf{w} = \frac{\mathbf{\hat{w}}}{J} = \left[ -\rho u \frac{1}{A} \frac{\partial A^c}{\partial \xi}, -\rho u \frac{1}{A} \frac{1}{A} \frac{\partial A^c}{\partial \xi}, -\rho u \left( E + \frac{p}{\rho} \right) \frac{1}{A} \frac{\partial A}{\partial \xi} \right]^T.
\]

The above vectors are identical to those presented in Section 3.2.

The KT numerical technique requires only the eigenvalues of the generalized flux Jacobian. Eq. (C.1) can be expressed as

\[
\frac{\partial \mathbf{\hat{q}}}{\partial t} + \hat{\mathbf{A}} \frac{\partial \mathbf{\hat{q}}}{\partial \xi} = \mathbf{\hat{w}},
\]

(C.18)

where \( \hat{\mathbf{A}} \) is the flux Jacobian given by

\[
\hat{\mathbf{A}} \equiv \frac{\partial \mathbf{f}}{\partial \mathbf{q}} = \begin{bmatrix}
0 & 1 & 0 \\
\frac{\gamma - 3}{2} u^2 & (3 - \gamma) u & (\gamma - 1) \\
u \left[ (\gamma - 1) u^2 - \gamma E \right] & \gamma E - \frac{3}{2} (\gamma - 1) u^2 & \gamma u
\end{bmatrix}.
\]

(C.19)

The gas equations of state were utilized in deriving the elements of the above matrix. Since the governing equations are solved in the fixed computational plane, the eigenvalues of the generalized flux Jacobian need to be obtained. Thus, Eq. (C.17) is written as

\[
\frac{\partial \mathbf{q}}{\partial \tau} + \mathbf{A} \frac{\partial \mathbf{q}}{\partial \xi} = \mathbf{w}.
\]

(C.20)

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By knowing the generalized conservation vector \( \mathbf{q} \) and the generalized flux vector \( \mathbf{f} \), the generalized flux Jacobian can be determined by applying the chain rule:

\[
\mathbf{f} = \frac{\xi \mathbf{q} + \xi_x \mathbf{f}}{J},
\]

\[
= f \left[ \mathbf{q} (\mathbf{q}), \mathbf{f} (\mathbf{q}) \right],
\]

\[
\mathbf{A} \equiv \frac{\partial \mathbf{f}}{\partial \mathbf{q}} = \frac{\partial f}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial \mathbf{q}} + \frac{\partial f}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial \mathbf{q}},
\]

\[
= \frac{\xi_x}{J} \mathbf{I} + \frac{\xi_x}{J} \frac{\partial \mathbf{f}}{\partial \mathbf{q}} J,
\]

\[
= \xi_x \mathbf{I} + \xi_x \mathbf{A},
\]

where \( \mathbf{I} \) is the identity matrix. Using the flux Jacobian \( \mathbf{A} \) given by Eq. (C.19) and rearranging terms, the generalized flux Jacobian is given by

\[
\mathbf{A} = \begin{bmatrix}
\xi_x & \xi_x & 0 \\
\gamma - 3 \left( U^c - \xi_x \right) u & U_c + \xi_x \left( 2 - \gamma \right) u & \xi_x (\gamma - 1) \\
(U_c - \xi_x) \left[ (\gamma - 1) u^2 - \gamma E \right] & \xi_x \gamma E - \frac{3}{2} (\gamma - 1) (U_c - \xi_x) u & \xi_x + \gamma (U_c - \xi_x)
\end{bmatrix}.
\]

The eigenvalues of the generalized flux Jacobian, Eq. (C.23), are found by solving the characteristic equation

\[
\det (\mathbf{A} - \mathbf{\lambda}) = 0,
\]

where \( \mathbf{\lambda} \) is the diagonal matrix of eigenvalues. The elements of this matrix were found to be

\[
\mathbf{\lambda} = \begin{bmatrix}
U^c & 0 & 0 \\
0 & U^c - \xi_x c & 0 \\
0 & 0 & U^c + \xi_x c
\end{bmatrix}.
\]

The eigenvalues of the generalized flux Jacobian matrix are both real and distinct; therefore, the corresponding eigenvectors are linearly independent and Eqs. (3.8)-(3.10) constitute a strictly hyperbolic system of PDEs [45].
Vita

Blaise H. Paul is a Louisiana native from the small city of Central in East Baton Rouge Parish. He enrolled at Baton Rouge Community College in 2001 before beginning his engineering career path in 2003 at Louisiana State University. In 2006, Blaise accepted an invitation to the Department of Mechanical Engineering’s Accelerated Master’s Program, also known as the 3–2 Program. Blaise was later married to Colleen Birke and earned his Bachelor of Science in Mechanical Engineering degree in 2007. He is a candidate for the Master of Science in Mechanical Engineering degree to be awarded in December 2008.